Multi-component supramolecular compounds containing hexaamminecobalt(III) cations and aromatic sulfonic acid derivatives

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Content

Table S1. $[Co(NH_3)_6]$-based compounds*

Nr.	Code in CCDC	Formula	Properties/ function of the $[Co(NH_3)_6]^{3+}$ cation	Reference
1.	BAKMAF	$\{[Co(NH_3)_6]_2(U_5C_{54}H_{84}N_6O_{51})\}_n$	Hydrogen-bonded network	X. Li, J. Lu, W. Mu, B. Chen, D. Luo, B. Liu, Y. Yang, H. Wei, S. Peng, *Inorg. Chim. Acta*, **2022**, 530, 120675, DOI: 10.1016/j.ica.2021.120675
2.	ADIYES	$[Co(NH_3)_6]_2(bpds)_3 \cdot 2dmso \cdot 5H_2O$	Hydrogen-bonded metal-complex host–guest properties	X.-Y. Wang, R. Justice, S. C. Sevov, *Inorg. Chem*., **2007**, 46, 4626, DOI: 10.1021/ic070324p
	ADIYIW	$[Co(NH_3)_6]_2(bpds)_3 \cdot 2dmf \cdot 2H_2O$		
	ADIYOC	$[Co(NH_3)_6]_2(bpds)_3 \cdot piperidine \cdot 2H_2O$		
	ADIYUI	$[Co(NH_3)_6]_2(bpds)_3 \cdot 2acetone \cdot 4H_2O$		
	AFIKOQ	$[Co(NH_3)_6]_2(bpds)_3 \cdot 2acetonitrile \cdot 4H_2O$		
	AFIKUW	$[Co(NH_3)_6]_2(bpds)_3 \cdot 2thf \cdot 4H_2O$		
3	AHIKUX	$[Co(NH_3)_6][Gd(nta)_2(H_2O)] \cdot 8H_2O$	Hydrogen-bonded network	S. M. Baldwin, M. E. Kastner, *Acta Cryst., C: Cryst. Struct. Comm*., **2002**, 58, m611, DOI: 10.1107/S0108270102019601
4	ASAWOH01	$[Co(NH_3)_6](adc)(Hadc) \cdot 2H_2O$	Hydrogen-bonded network	R. W. Seidel, R. Goddard, V. Gramm, U. Ruschewitz, *Z. Naturforsch., B: Chem. Sci.*, **2014**, 69, 277, DOI: 10.5560/ZNB.2014-3272
5	ASAWUN	$[Co(NH_3)_6](Hadc)Cl_2 \cdot H_2O$	Hydrogen-bonded network	I. Stein, U. Ruschewitz. *Z. Naturforsch., B: Chem. Sci*. **2011**, 66, 471
6	BANXOD	$[Co(NH_3)_6]_5[Ag_8Ni_6(pen)_{12}Cl]_3 \cdot 197H_2O$	Hydrogen-bonded network	P. J. M. W. L. Birker, J. Reedijk, G. C. Verschoor, *Inorg. Chem*., **1981**, 20, 2877, DOI: 10.1021/ic50223a027
7	BEFWAO	$[Co(NH_3)_6]_2[Th(ox)_5] \cdot 4H_2O$	Hydrogen-bonded network	C. Tamain, M. Autillo, D. Guillaumont, L. Guérin, R. E. Wilson, C. Berthon, *Inorg. Chem*., **2022**, 61, 12337, DOI: 10.1021/acs.inorgchem.2c01674
	BEFWES	$[Co(NH_3)_6]_2[U(ox)_5] \cdot 4H_2O$		
	BEFWIW	$[Co(NH_3)_6]_2[Np(ox)_5] \cdot 4H_2O$		
	BEFWOC	$[Co(NH_3)_6]_2[Pu(ox)_5] \cdot 4H_2O$		
8	CACDAO	$[Co(NH_3)_6](BH_4)_2$	High hydrogen densities and low decomposition temperatures	E. Roedern, T. R. Jensen, *Inorg. Chem*., **2015**, 54, 10477, DOI: 10.1021/acs.inorgchem.5b01959
	CACDES	$[Co(NH_3)_6](BH_4)_{2-x}Cl_x$		
9	CAFWEM	$\{[Co(NH_3)_6][UO_2(mma)(dmma)]\}_2Cl_2 \cdot 6H_2O$	Hydrogen-bonded network	Y. Zhang, D .Collison, F. R. Livens, M. Helliwell, F. Heatley, A. K. Powell, S. Wocadlo, H. Eccles, *Polyhedron*, **2002**, 21,

				81, DOI: 10.1016/S0277-5387(01)00965-2
10	CANYAS	$[Co(NH_3)_6]Cl(pht)_2 \cdot 3H_2O$	Building block for larger supramolecular assemblies	R. P. Sharma, R. Bala, R. Sharma, B. M. Kariuki, U. Rychlewska, B. Warzajtis, *J. Mol. Struct*., **2005**, 748, 143, DOI: 10.1016/j.molstruc.2005.03.028
	CANYEW	$Na[Co(NH_3)_6](benz)_4 \cdot H_2O$		
11	CAXPUP	$[Co(NH_3)_6][Yb(dipic)_3] \cdot 8.5H_2O$	Hydrogen-bonded network	J. M. Harrowfield, I. Ling, B. W. Skelton, A. N. Sobolev, A. H. White, *Aust. J. Chem.*, **2017**, 70, 485, DOI: 10.1071/CH16584
	CAXQEA	$[Co(NH_3)_6][La(dipic)_3] \cdot 8.5H_2O$		
	CAXQEA01	$[Co(NH_3)_6][La(dipic)_3] \cdot 8.5H_2O$		
	CAXQOK	$[Co(NH_3)_6][Ce(dipic)_3] \cdot 10H_2O$		
	CAXQUQ	$[Co(NH_3)_6][Gd(dipic)_3] \cdot 10H_2O$		
	CAXXEH	$[Co(NH_3)_6][Nd(dipic)_3] \cdot 10H_2O$		
	CAXXIL	$[Co(NH_3)_6][Eu(dipic)_3] \cdot 10H_2O$		
	CAXXOR	$[Co(NH_3)_6][Gd(dipic)_3] \cdot 10H_2O$		
	CAXYAE	$[Co(NH_3)_6][Ho(dipic)_3] \cdot 10H_2O$		
	CAXYIM	$[Co(NH_3)_6][Gd(dipic)_3] \cdot 8H_2O$		
12	CIFCUQ	$[Co(NH_3)_6]_3[Nb_6O_{19}H_2]$		R. P. Bontchev, E. L. Venturini, M. Nyman, *Inorg. Chem*., **2007**, 46, 4483, DOI: 10.1021/ic0624118
13	CITQOO	$(NH_4)_2\{Co(NH_3)_6\}_2[Am_3(Citr)_4(OH)(H_2O)_2] \cdot nH_2O$	Hydrogen-bonded network	G. Andreev, N. Budantseva, A. Fedoseev, *Inorg. Chem. Comm*., **2019**, 99, 160, DOI: 10.1016/j.inoche.2018.11.022
14	DAJWAM	$[Co(NH_3)_6]_3$-$[Fe(mal)_3] \cdot 5H_2O$	Hydrogen-bonded network	W. Clegg, *Acta Cryst., C: Cryst. Struct. Comm*., **1985**, 41, 1164, DOI: 10.1107/S0108270185006990
15	DERYEF	$Li[Co(NH_3)_6][Pu(mal)_4] \cdot 5H_2O$	Hydrogen-bonded network	M. S. Grigoriev, N. N. Krot, A. A. Bessonov, K. A. Lyssenko, *Acta Crystallogr. Sect. E Struct. Rep. Online*, **2006**, 62, m2889, DOI: 10.1107/S1600536806041328
16	DILBOP	$[Co(NH_3)_6][Nd(citr)_2] \cdot 8H_2O$	Hydrogen-bonded network	S. Bouhlassa, R. Guillaumont, *Bulletin de la Societe Chimique de France*, **1984**, 1-2, 12.
17	EDTACO	$[Co(NH_3)_6][Na(edta)] \cdot 3.5H_2O$	Hydrogen-bonded network	E. O. Schlemper, *Journal of Crystal and Molecular Structure*, **1977**, 7, 81, DOI: 10.1007/BF01369834
18	EGABAR	$[Co(NH_3)_6]_2[Cd_8(ox)_{11}(H_2O)_4] \cdot 8H_2O$	Template in the formation of metal–organic frameworks (MOFs) with the corresponding sizes of pore	Q.-H. Pan, R.-J. Tian, S.-J. Liu, Q.-H. Wu, Y.-Y. Zhu, Q. Chen, X.-Y. Ren, T.-L. Hu, *Chinese Chemical Letters*, **2013**, 24, 861, DOI: 10.1016/j.cclet.2013.06.025

19	EXEHIY	$[Co(NH_3)_6]_3[Cu_4(OH)(CO_3)_8]\cdot 2H_2O$	Hydrogen-bonded network	B. F. Abrahams, M. G. Haywood, R. Robson, *Chem. Commun*., **2004**, 938, DOI: 10.1039/b316925a
20	EYAQEA	$[Co(NH_3)_6]Cl(mes)_2$	Hydrogen bonding network	R. P. Sharma, R. Bala, R. Sharma, P. Venugopalan, *J. Mol. Struct*., **2004**, 694, 229, DOI: 10.1016/j.molstruc.2004.03.040
21	FECGAX	$[Co(NH_3)_6](ClO_4)_3$	Phase transition, hydrogen bonding network	N. Gorska, A. Inaba, Y. Hirao, E. Mikuli, K. Holderna-Natkaniec, *RSC Advances*, **2012**, 2, 4283, DOI: 10.1039/c2ra01184k
	FECGAX01	$[Co(NH_3)_6](ClO_4)_3$		
22	FIRJIZ	$\{[Co(NH_3)_6][UO_2(dmma)_2]Cl\}_2\cdot 7H_2O$	Effects on the aggregation of the uranyl complexes	Y. Zhang, D. Collison, F.R. Livens, M. Helliwell, H. Eccles, N. Tinker, *J. Alloys Compd*., **1998**, 271, 139, DOI: 10.1016/S0925-8388(98)00041-3
23	GEFGOO	$[Co(NH_3)_6]Cl_2SeCN$	Hydrogen bonding network	R. P. Sharma, R. Bala, R. Sharma, P. Venugopalan, *CrystEngComm*, **2006**, 8, 215, DOI: 10.1039/b516629b
	GEWNIJ	$[Co(NH_3)_6]Cl(oaca)_2\cdot H_2O$	Hydrogen bonding network	M. Fonari, V. Kravtsov CCDC 2167981: Experimental Crystal Structure Determination, 2023.
	GEWNOP	$[Co(NH_3)_6]Cl(dmb)_2\cdot 2H_2O$	Hydrogen bonding network	M. Fonari, V. Kravtsov CCDC 2167982: Experimental Crystal Structure Determination, 2023.
24	GEZZIU	$[Co(NH_3)_6][las]_3\cdot 3.3H_2O$	Hydrogen bonding network	F. Takusagawa, J. Shaw, G.W. Everett, *Inorg. Chem*., **1988**, 27, 3107, DOI: 10.1021/ic00291a013
25	HEQNAT	$[Co(NH_3)_6][B(CO_2)_2(CO_2H)_2]\cdot 2H_2O$		E. Bernhardt, D. J. Brauer, M. Finze, H. Willner, *Angew. Chem., Int. Ed*., **2006**, 45, 6383, DOI: 10.1002/anie.200601870
26	HOSFUS	$[Co(NH_3)_6]_4[Ce(O_2)(CO_3)_3]_2(CO_3)_2\cdot 12H_2O$	Hydrogen bonding network	N.-P. Pook, A. Adam, *ZAAC*, **2014**, 640, 2931, DOI: 10.1002/zaac.201400376
27	JACREN	$[Co(NH_3)_6][Ce(ox)_3(H_2O)]\cdot H_2O$	Template to design 3D open frameworks with zeolite topologies	R. Tian, F. Wang, Ch. Du, L. Feng, Y. Liu, C. Zhang, Q. Pan, *Chemical Research in Chinese Universities*, **2014**, 30, 889, DOI: 10.1007/s40242-014-4178-8
28	KEKZUX	$[Co(NH_3)_6]_2[Cu(ox)_2]_3$		D. P. Domonov, N. V. Kuratieva, S. I. Pechenyuk, *J. Struct. Chem*., **2011**, 52, 358, DOI: 10.1134/S0022476611020168
	KEKZUX01	$[Co(NH_3)_6]_2[Cu(ox)_2]_3$		
29	KEQGOD	$[Co(NH_3)_6]_3(Hhbsa)_8Cl\cdot 13H_2O$	Hydrogen-bonded network	R. P. Sharma, R. Bala, R. Sharma, A. D. Bond, *Acta Crystallogr. Sect. E Struct. Rep. Online,* **2006**, 62, m2113, DOI: 10.1107/S1600536806029989
30	KUTCEH	$[Co(NH_3)_6][NpO_2(ox)_2]\cdot 3H_2O$		M. S. Grigor'ev, N. A. Baturin, L. L. Regel', N. N. Krot,

	KUTCIL	$[Co(NH_3)_6][NpO_2(ox)_2]\cdot 4H_2O$		*Radiokhimiya*, **1991**, 33, 19
31	LECKIO	$[Co(NH_3)_6](xdsa)_{1.5}\cdot 2H_2O$	A host network for selective uptake of guest molecules	S. A. Dalrymple, G. K. H. Shimizu, *Chem. Commun*., **2006**, 956, DOI: 10.1039/b515735h
	LECKOU	$[Co(NH_3)_6](xdsa)_{1.5}(an)\cdot 3H_2O$		
32	MANGUF	$[Co(NH_3)_6]_3[Zn_8(HPO_4)_8(PO_4)_2](PO_4)$ (ZnPO-CJ68)	A template for designing microporous frameworks	Y. Han, Y. Li, J. Yu, Q. Pan, R. Xu, *Eur. J. Inorg. Chem*., **2012**, 36, DOI: 10.1002/ejic.201100816
33	MIBCAC	$[Co(NH_3)_6]_5[Cu_6Cu_8(miba)_{12}Cl]\cdot nH_2O$		P. J. M. W. L. Birker, *Inorg. Chem*., **1979**, 18, 3502, DOI: 10.1021/ic50202a042
34	MIWTUJ	$[Co(NH_3)_6]_2(adc)_3\cdot 3H_2O$	Hydrogen-bonded network	R. W. Seidel, R. Goddard, V. Gramm, U. Ruschewitz, *Zeitschrift fur Naturforschung, B: Chemical Sciences*, **2014**, 69, 277, DOI: 10.5560/ZNB.2014-3272
35	CANYAS01	$[Co(NH_3)_6]Cl(Hpht)\cdot 3H_2O$	Hydrogen-bonded network, inhibitory potential against bacterial cancer in plants	M. Darii, E. S. Beleaev, V. Ch. Kravtsov, P. Bourosh, Y. Chumakov, J. Hauser, S. Decurtins, S.-X. Liu, O. Sultanova, S. G. Baca, *New J. Chem*., **2022**, 46, 11404, DOI: 10.1039/D2NJ01655A
	MEHRUQ	$[Co(NH_3)_6]Cl_3\cdot 2(phen)\cdot 3H_2O$		
	MEHSAX	$[Co(NH_3)_6](Hbdc)(bdc)\cdot 3H_2O$		
	MEHSEB	$[Co(NH_3)_6]Cl_2(Hpht)\cdot 3H_2O$		
	MEHSOL	$[Co(NH3)_6]Cl(2,3\text{-}pdc)\cdot H_2O$		
	MEHSUR	$[Co(NH_3)_6]Cl(sb)\cdot 4H_2O$		
	MEHTAY	$[Co(NH_3)_6]_2(sb)_3\cdot EtOH\cdot 2{,}5H_2O$		
	MEHTEC	$[Co(NH_3)_6][Co(3,5\text{-}pdc)_2(H_2O)_4]Cl\cdot 3H_2O$		
	MEHTIG	$[Co(NH_3)_6]_{11}[Co(2,5\text{-}pdc)_3]_8Cl\cdot 84H_2O$		
36	NAKZUV	$[Co(NH_3)_6](dipic)Cl\cdot 2H_2O$	Hydrogen bonding network	P. A. Brayshaw, A. K. Hall, W. T. A. Harrison, J. M. Harrowfield, D. Pearce, T. M. Shand, B. W. Skelton, C. R. Whitaker, A. H. White, *Eur. J. Inorg. Chem*., **2005**, 1127, DOI: 10.1002/ejic.200400863
	NALBAE	$[Co(NH_3)_6][La(dipic)_3]\cdot 5H_2O$		
	NALBEI	$[Co(NH_3)_6][Ce(dipic)_3]\cdot 5H_2O$		
	NALBIM	$[Co(NH_3)_6][Pr(dipic)_3]\cdot 5H_2O$		
	NALBOS	$[Co(NH_3)_6][Pr(dipic)_3]\cdot 10H_2O$		
	NALBUY	$[Co(NH_3)_6][Sm(dipic)_3]\cdot 10H_2O$		
	NALCAF	$[Co(NH_3)_6][Tb(dipic)_3]\cdot 10H_2O$		
	NALCEJ	$[Co(NH_3)_6][Er(dipic)_3]\cdot 10H_2O$		
	NALCIN	$[Co(NH_3)_6][Y(dipic)_3]\cdot 10H_2O$		
	NALCOT	$[Co(NH_3)_6][Tm(dipic)_3]\cdot 8.5H_2O$		
	NALCUZ	$[Co(NH_3)_6][Lu(dipic)_3]\cdot 8.5H_2O$		

37	NALBAE01	$[Co(NH_3)_6][La(dipic)_3]\cdot 5H_2O$	Hydrogen bonding network	J. M. Harrowfield, I. Ling, B. W. Skelton, A. N. Sobolev, A. H. White, *Aust. J. Chem*., **2017**, 70, 485, DOI: 10.1071/CH16584
	NALBEI01	$[Co(NH_3)_6][Ce(dipic)_3]\cdot 5H_2O$		
	NALBIM01	$[Co(NH_3)_6][Pr(dipic)_3]\cdot 5H_2O$		
	NALCAF01	$[Co(NH_3)_6][Tb(dipic)_3]\cdot 10H_2O$		
	NALCIN01	$[Co(NH_3)_6][Y(dipic)_3]\cdot 10H_2O$		
	NALCOT01	$[Co(NH_3)_6][Tm(dipic)_3]\cdot 8.5H_2O$		
	NALCUZ01	$[Co(NH_3)_6][Lu(dipic)_3]\cdot 8.5H_2O$		
38	NALBIM02	$[Co(NH_3)_6][Pr(dipic)_3]\cdot 5H_2O$		B. W. Skelton, J. M. Harrowfield, A. H. White, *CSD Communication*, **2017**
39	NANCUB	$[Co(NH_3)_6](NpO_2mal)_2OH\cdot H_2O$		I.A. Charushnikova, N.N. Krot, I.N. Polyakova, *Radiokhimiya*, **2004**, 46, 318
	NANDAI	$[Co(NH_3)_6](NpO_2mal)_2NO_3\cdot H_2O$		
40	NEKHOE	$[Co(NH_3)_6]_4[UO_2(CO_3)_3]_3\cdot H_2O$	Hydrogen bonding network	M. M. F. Pyrch, J. L. Bjorklund, J. M. Williams, M. Kasperski, S. E. Mason, T. Z. Forbes, *Inorg. Chem*., **2022**, 61, 15023, DOI: 10.1021/acs.inorgchem.2c01982
	NEKHUK	$[Co(NH_3)_6]_2[UO_2(CO_3)_3]CO_3$		
	NEKJAS	$[Co(NH_3)_6]Cl(CO_3)$		
	NEKJEW	$[Co(NH_3)_6]_2[UO_2(CO_3)_3]Cl_2$		
41	NEYBUQ	$[Co(NH_3)_6](BF_4)_3$	Phase transitions	N. Gorska, A. Inaba, Y. Hirao, E. Mikuli, *J. Coord. Chem*., **2013**, 66, 1238, DOI: 10.1080/00958972.2013.777834
	NEYBUQ01	$[Co(NH_3)_6](BF_4)_3$		
42	NEYHOP	$[Co(NH_3)_6]Cl_2(Hox)\cdot H_2O$	Hydrogen bonding network	R. Bala, R.P. Sharma, U. Sharma, A.D. Burrows, K. Cassar, *J. Mol. Struct*., **2007**, 832, 156, DOI: 10.1016/j.molstruc.2006.08.028
43	OKOCAS	$\{[Co(NH_3)_6]NpO_2(pht)_2\cdot 2H_2O\}_n$	Hydrogen bonding network; supramolecular assembly	I. A. Charushnikova, N. N. Krot, Z. A. Starikova, *Radiokhimiya*, **2001**, 43, 438
44	OTEXER	$[Co(NH_3)_6][Au(CN)_4]_3\cdot 4H_2O$	Hydrogen bonding network	A. R. Geisheimer, J. E. C. Wren, V. K. Michaelis, M. Kobayashi, K. Sakai, S. Kroeker, D. B. Leznoff, *Inorg. Chem*., **2011**, 50, 1265, DOI: 10.1021/ic101782v
45	PEFRIC	$[Co(NH_3)_6]Cl(mes)_2$	Hydrogen bonding network	R. P. Sharma, R. Bala, R. Sharma, K. N. Singh, V. Ferretti, *J. Mol. Struct.*, **2006**, 784, 117, DOI: 10.1016/j.molstruc.2005.08.009
46	PEWCIG	$[Co(NH_3)_6]_4[Mo_4O_{12}(ox)_4][MoO_3(ox)H_2O)]_2\cdot 10H_2O$	Hydrogen bonding network; supramolecular assembly	M. Cindrić, V. Stilinović, M. Rubčić, G. Medak, D. Š. Jung, V. Vrdoljak, *CrystEngComm*, **2018**, 20, 1889, DOI: 10.1039/C7CE02205K
	PEWCOM	$[Co(NH_3)_6]_2[Mo_4O_{11}(ox)_4(H_2O)]\cdot 6H_2O$		

47	PUJSIZ	$[Co(NH_3)_6]_3[Ti_4O_6(Hcit)_3(cit)]\cdot 20H_2O$	cytotoxicity towards the ovarian cells	N. Engelberg, A. Bino, E. Y. Tshuva, *Inorg. Chim. Acta*, **2020**, 503, 119429, DOI: 10.1016/j.ica.2020.119429
48	QAGJUF	$[Co(NH_3)_6]_2K[Nd_3(cit)_4(H_2O)_3]\cdot 18H_2O$		A. M. Fedosseev, M. S. Grigoriev, N. A. Budantseva, D. Guillaumont, C. Le Naour, E. Simoni, C. Den Auwer, P. Moisy, *Comptes Rendus Chimie*, **2010**, 13, 839, DOI: 10.1016/j.crci.2010.04.018
	QAGKAM	$[Co(NH_3)_6]_2K[Am_3(cit)_4(H_2O)_3]\cdot 18H_2O$		
49	QUTGUJ	$[Co(NH_3)_6][Co(CO)_4]_2$	$[Co(NH_3)_6]^{2+}$	T. G. Müller, F. Kraus, *Acta Crystallog. Section E: Crystallog. Commun.*, **2015**, 71, 1418, DOI: 10.1107/S2056989015020290
50	QUTNIC	$[Co(NH_3)_6][Fe(CN)_5(CO)]\cdot 3H_2O$		J. Jiang, A. Acunzo, S. A. Koch, *JACS*, **2001**, 123, 12109, DOI: 10.1021/ja016434r
51	RAJNIZ	$[Co(NH_3)_6]C_{60}\cdot 6NH_3$		H. Brumm, M. Jansen, *ZAAC*, **2001**, 627, 1433, DOI: 10.1002/1521-3749(200107)627:7<1433::AID-ZAAC1433>3.0.CO;2-H
52	RATDUL	$[Co(NH_3)_6]$-mer,trans-$[Co(NO_2)_3(NH_3)_2(CH_3)]_2$-trans-$[Co(NO_2)_4(NH_3)_2]$	Hydrogen-bonded network	P. Kofod, P. Harris, S. Larsen, *Inorg. Chem.*, **1997**, 36, 2258, DOI: 10.1021/ic961264i
53	REMMEC	$[Co(NH_3)_6][Hg_2(SCN)_7]$	Hydrogen-bonded network	R. Bala, R. P. Sharma, R. Sharma, B. M. Kariuki, *Inorg. Chem. Commun.*, **2006**, 9, 852, DOI: 10.1016/j.inoche.2006.05.003
54	RENVIQ	$[Co(NH_3)_6]Cl(pnb)_2$	Hydrogen bonding network	R. P. Sharma, R. Bala, R. Sharma, J. Perez, D. Miguel, *J. Mol. Struct.*, **2006**, 797, 49, DOI: 10.1016/j.molstruc.2006.03.046
55	RORNER	$[Co(NH_3)_6][Sb(H_3guo)_2]\cdot 9H_2O$		P. Klufers, P. Mayer, *ZAAC*, **1997**, 623, 1496, DOI: 10.1002/zaac.19976231003
56	SANCOA	$\{[Co(NH_3)_6][NpO_2mal]_2\cdot Hmal\}_n$	Hydrogen bonding network; supramolecular assembly	M. S. Grigor'ev, I. A. Charushnikova, Z. A. Starikova, N. N. Krot, I. N. Polyakova, *Radiokhimiya*, **2004**, 46, 212
57	SEDFEP	$[Co(NH_3)_6](bppa)\cdot 4H_2O$	Hydrogen bonding network	Ch. Heering, B. Nateghi, Ch. Janiak, *Crystals*, **2016**, 6, 22, DOI: 10.3390/cryst6030022
58	SICHAO	$[Co(NH_3)_6][Bi(H_3guo)_2]\cdot 9H_2O$	Hydrogen-bonded network	P. Klufers, P. Mayer, *ZAAC*, **2007**, 633, 903, DOI: 10.1002/zaac.200700054
59	SIWZAZ	$[Co(NH_3)_6][Co(hbg)]Cl\cdot 10H_2O$	Hydrogen-bonded network	C. Ming-Qin, X. Jun-Xing, Z. Hua-Ling J. Huaxue (Chin.) (Chin. J. Struct. Chem.) **1991**,10,1
60	SUTYOW	$[Co(NH_3)_6][Yb(nta)_2(H_2O)]\cdot 8H_2O$	Hydrogen-bonded	A. M. Fedosseev, M. S. Grigoriev, N. A. Budantseva, D.

	SUTYUC	$[Co(NH_3)_6][Nd(nta)_2(H_2O)]\cdot 8H_2O$	network	Guillaumont, C. Le Naour, E. Simoni, C. Den Auwer, P. Moisy, *Comptes Rendus Chimie*, **2010**, 13, 839, DOI: 10.1016/j.crci.2010.04.018
	SUTZAJ	$[Co(NH_3)_6][Am(nta)_2(H_2O)]\cdot 8H_2O$		
61	TAPWIR	$\{Na[Co(NH_3)_6](fbenz)_4\cdot H_2O\}_n$	Hydrogen bonding network, supramolecular assembly	R. P. Sharma, R. Bala, R. Sharma, A. D. Bond, *Acta Crystallog., Section C: Cryst. Struct. Commun.,* **2005**, 61, m356, DOI: 10.1107/S0108270105018500
62	TUTMAZ	$\{Cd_2[Co(NH_3)_6](btc)_2Cl\cdot 3H_2O\}_n$	Hydrogen bonding network; supramolecular assembly; proton conduction	F.-X. Wang, G.-J. Ren, R.-J. Tian, L.-J. Feng, Y.-H. Yang, Y.-Y. Deng, Q.-H. Pan, *Jiegou Huaxue*, **2020**, 39, 1337, DOI: 10.14102/j.cnki.0254-5861.2011-2609
63	VAFKOD	$[Co(NH_3)_6]_2(sms)_2\cdot 6H_2O$	Hydrogen-bonded network	S. A. Dalrymple, M. Parvez, G. K. H. Shimizu, *Inorg. Chem*., **2002**, 41, 6986, DOI: 10.1021/ic025627s
64	VUCCON	$\{[Co(NH_3)_6][La(mal)_2]_3\cdot 6H_2O\}_n$	Hydrogen bonding network, supramolecular assembly	I. A. Charushnikova, N. N. Krot, V. I. Makarenkov, Z. A. Starikova, *Radiokhimiya*, **2014**, 56, 364, DOI: 10.1134/S106636221404002X
	VUCCUT	$\{[Co(NH_3)_6][Ce(mal)_2]_3\cdot 6H_2O\}_n$		
	VUCDAA	$\{[Co(NH_3)_6][Nd(mal)_2]_3\cdot 6H_2O\}_n$		
	VUCDEE	$\{[Co(NH_3)_6][Pr(mal)_2]_3\cdot 6H_2O\}_n$		
	VUCDII	$\{[Co(NH_3)_6]_2[Tb_3(mal)_7(Hmal)(H_2O)_4]\cdot 6H_2O\}_n$		
	VUCDOO	$\{[Co(NH_3)_6]_2[Er_3(mal)_7(Hmal)(H_2O)_4]\cdot 6H_2O\}_n$		
	VUCDUU	$\{[Co(NH_3)_6]_2[Tm_3(mal)_7(Hmal)(H_2O)_4]\cdot 6H_2O\}_n$		
	VUCFAC	$\{[Co(NH_3)_6]2[Ho_3(mal)_7(Hmal)(H_2O)_4]\cdot 6H_2O\}_n$		
65	WABXUT	$\{[Co(NH_3)_6]Cl(pipes)(H_2O)_6\}_n$	Hydrogen bonding network, supramolecular assembly	D. S. Reddy, S. Duncan, G. K. H. Shimizu, *Angew. Chem., Int. Ed*., **2003**, 42, 1360, DOI: 10.1002/anie.200390348
	WABYAA	$\{[Co(NH_3)_6](nds)_{1.5}(H_2O)_2(dioxane)\}_n$		
66	WEHBIV	$[Co(NH_3)_6][PuO_2(ox)_2]\cdot 3H_2O$	Hydrogen-bonded network	M. S. Grigor'ev, M. Yu. Antipin, N. N. Krot, A. A. Bessonov, *Radiokhimiya*, **2005**, 47, 419
67	WEHBUH	$[Co(NH_3)_6][NpO_2(ox)_2]\cdot 3H_2O$	Hydrogen-bonded network	I. A. Charushnikova, N. N. Krot, I. N. Polyakova, *Radiokhimiya*, **2005**, 47, 495
68	WEXRIB	$[Co(NH_3)_6](mes)_3$	Hydrogen bonding network	R. Bala, R. P. Sharma, A. D. Bond, *J. Mol. Struct*., **2007**, 830, 198, DOI: 10.1016/j.molstruc.2006.07.016
69	WEXTID	$[Co(NH_3)_6]Cl(tart)\cdot H_2O$	Hydrogen bonding network,	R. Bala, R.P. Sharma, P. Venugopalan, W.T.A. Harrison, *J. Mol. Struct*., **2007**, 830, 8, DOI:

			supramolecular assembly	10.1016/j.molstruc.2006.06.024
70	WIRLAM	$[Co(NH_3)_6][Cu(ta)_2Cl(H_2O)]$	Hydrogen bonding network	G. Pascu, C. Deville, S. E. Clifford, L. Guenée, C. Besnard, K. W. Krämer, S.-X. Liu, S. Decurtins, F. Tuna, E. J. L. McInnes, R. E. P. Winpenny, A. F. Williams, *Dalton Trans.*, **2014**, 43, 656, DOI: 10.1039/C3DT51838H
71	WUBDEF	$[Co(NH_3)_6]_2[B_4O_5(OH)_4]_3 \cdot 11H_2O$	Hydrogen bonding network	M. A. Altahan, M. A. Beckett, S. J. Coles, P. N. Horton, *J. Mol. Struct*., **2020**, 1200, 127071, DOI: 10.1016/j.molstruc.2019.127071
72	WUYVET	$[Co(NH_3)_6][Mn(CN)_6]$	Hydrogen bonding network	H. G. Visser, W. Purcell, *Acta Crystallogr. Sect. E Struct. Rep. Online*, **2008**, 64, i76, DOI: 10.1107/S1600536808032881
73	XATROA	$[Co(NH_3)_6][NpO_2(Hmal)_2(H_2O)_3](Hmal)_2 \cdot H_2O$	Hydrogen bonding network	I. A. Charushnikova, N. N. Krot, Z. A. Starikova, *Radiokhimiya*, **2004**, 46, 521
74	XECQUT	$[Co(NH_3)_6]_3[Co(ox)_3]_2Cl \cdot 12H_2O$	Hydrogen bonding network	R. Tian, Y. Yan, C. Zhang, L. Wang, Q. Pan, *Acta Crystallogr. Sect. E Struct. Rep. Online*, **2012**, 68, m914, DOI: 10.1107/S1600536812026414
75	XEDNAV	$[Co(NH_3)_6]_2(ox)_3 \cdot 4H_2O$	Hydrogen bonding network	M. Gorol, N.C. Mosch-Zanetti, M. Noltemeyer, H.W. Roesky, *ZAAC*, **2000**, 626, 2318, DOI: 10.1002/1521-3749(200011)626:11<2318::AID-ZAAC2318>3.0.CO;2-W
76	XEDNAV01	$[Co(NH_3)_6]_2(ox)_3 \cdot 4H_2O$	Hydrogen-bonded network	D. P. Domonov, N. V. Kuratieva, S. I. Pechenyuk, *J. Struct. Chem*., **2011**, 52, 358, DOI: 10.1134/S0022476611020168
	XEDNAV02	$[Co(NH_3)_6]_2(ox)_3 \cdot 4H_2O$		
77	YAVZUR	$[Co(NH_3)_6](np)_3 \cdot 4H_2O$	Hydrogen bonding network	R. P. Sharma, R. Bala, R. Sharma, P. Venugopalan, *J. Mol. Struct*., **2005**, 752, 170, DOI: 10.1016/j.molstruc.2005.06.007
78	YOMNOF	$[Co(NH_3)_6][RuN(etgl)_2]_3$		O. Halevi, B. Bogoslavsky, D. Grinstein, F. Tibika-Apfelbaum, A. Bino, *Inorg. Chim. Acta*, **2014**, 421, 228, DOI: 10.1016/j. ica.2014.06.001
79	YUDJOY	$K[Co(NH_3)_6][Ce(O_2)(edta)]_2 \cdot 7H_2O$	Hydrogen bonding network	N.-P. Pook, A. Adam, *ZAAC*, **2014**, 640, 2931, DOI: 10.1002/zaac.201400376
80	ZZZBKD	$[Co(NH_3)_6]_5[Cu_{14}(D\text{-}Pen)_{12}Cl]_3 \cdot xH_2O$	Hydrogen bonding network	P. J. M. W. L. Birker, H. C. Freeman, *JACS*, **1977**, 99, 6890, DOI: 10.1021/ja00463a019
81	QECTEB	$[Co(NH_3)_6][Co(ox)_3] \cdot 3H_2O$	Hydrogen bonding network	E. Filatov, V. Lagunova, I. Kochetygov, P. Plyusnin, N. Kuratieva, G. Kostin, S. Korenev, *Acta Cryst. B: Struct. Sci., Crystal Engineering and Materials*, **2022**, 78, 537, DOI:
	QECTOL	$K_3[Co(NH_3)_6][Ir(ox)_3]_2 \cdot 6H_2O$		

				10.1107/S205252062200405X

∗ A search was conducted in CSD version 5.45 (Nov 2023) [F. H. Allen, *Acta Crystallogr. B*, 2002, **58**, 380] for $[Co(NH_3)_6]$-based compounds, employing the $[Co(NH_3)_6]$ cation drawing.

adc^{2-} = acetylenedicarboxilat; bdc^{2-} = diphenyl-4,4′-dicarboxylate; $benz^{-}$ = benzoate; $bpds^{2-}$ = 4,4′ biphenyldisulfonate; $bppa^{3-}$ =4-phosphono-biphenyl-4′-carboxylate; btc = 1,3,5-benzenetricarboxylate; $citr^{3-}$ = citrate; $dipic^{2-}$ = dipicolinate; $dmma^{2-}$ = dimethylmalonate; dmp^{-} - 2-(2,3-dimethylanilino)benzoate; D-Pen = D-Penicillamine; etgl = ethylene glycol; $fbenz^{-}$ = 4-fluorobenzoate; guo = guanosine; hbg = *o*-hydroxybenzylglycinate; $hbsa^{2-}$ = 4-hydroxybenzenesulfonate; las = lasalocid A; mal^{2-} = malonate; mes^{-} = methanesulfonate; mma^{2-} = methylmalonate; $miba^{2-}$ = a-mercaptoisobutyrate; nds^{2-} = 2,6-naphthalenedisulfonate; np^{-} = nitrophenolate; nta^{3-} = nitrilotriacetate; ox^{2-} = oxalate; pen^{2-} = penicillamine; pht^{2-} = *o*-phthalate; an = aniline; phen = 1,10-phenanthroline, pdc^{2-} = 2,3-/2,5-/3,5-pyridinedicarboxylate, $pipes^{2-}$ = 1,4-piperazine bis(ethanesulfonate); pnb^{-} = *p*-nitrobenzoate; sb^{2-} = 4-sulfobenzoate; sms^{3-} = trisulfonated mesitylene; $tart^{2-}$ = tartrate; $xdsa^{-}$ = α,α'-para-xylenedisulfonate; $oaca^{-}$ - 4-amino-1,2,5-oxadiazole-3-carboxylate

Table S2. Crystal data and details of structural determinations for **1**-**7**

	1	**2**	**3**	**4**
Formula	$C_{20}H_{35}CoN_{10}O_{12}S_4$	$C_{14}H_{32}ClCoN_{10}O_6S_2$	$C_7H_{24}ClCoN_6O_9S$	$C_7H_{54}Cl_2Co_2N_{12}O_{16}S_2$
M_r/g mol^{-1}	794.75	594.99	462.76	815.50

T/K	293(2)	293(2)	293(2)	293(2)
Cryst. system	Orthorhombic	Triclinic	Orthorhombic	Triclinic
Space group	*Fddd*	*P*-1	*Pnma*	*P*-1
a/Å	14.9159(12)	7.4363(6)	25.0699(10)	7.4383(5)
b/Å	18.4135(9)	8.2733(6)	7.2512(4)	12.0736(9)
c/Å	22.7514(13)	11.5486(14)	10.8265(6)	19.2979(12)
α/°	90	110.849(9)	90	100.100(6)
β/°	90	94.899(8)	90	98.038(6)
γ/°	90	90.864(6)	90	91.656(6)
V/Å^3	6248.8(7)	660.76(11)	1968.12(17)	1686.9(2)
Z	8	1	4	2
D_{calcd} / mg/m^3	1.690	1.495	1.562	1.605
μ / mm^{-1}	0.893	0.957	1.164	1.341
F(000)	3296	310	960	859
Crystal size / mm^3	0.500 x 0.400 x 0.300	0.500x0.160x0.050	0.500x0.400x0.250	0.500x0.04x0.03
Theta range for data collection / °	3.210 - 26.234	3.188 – 25.247	3.079 – 25.499	2.999 – 25.049
Index ranges	$-18\leq h\leq 14$, $-22\leq k\leq 21$, $-14\leq l\leq 28$	$-8\leq h\leq 8$, $-9\leq k\leq 9$, $-13\leq l\leq 12$	$-30\leq h\leq 11$, $-8\leq k\leq 8$, $-8\leq l\leq 13$	$-8\leq h\leq 8$, $-14\leq k\leq 7$, $-22\leq l\leq 22$
Refls collected/independent	3991/1576 (R_{int}=0.0222)	4513/2364 (R_{int}=0.0217)	4450/1978 (R_{int}=0.0241)	10656/5962 (R_{int}=0.0477)
Completeness to theta / % (θ = 25.50)	99.4	99.5	99.5	99.7
Data/restrains/parameters	1576 / 24 / 182	2364 / 0 / 160	1978 / 6 / 140	5962 / 9 / 410
Goodness-of-fit on F^2	1.000	1.003	1.026	0.852
Final R_1, wR_2	R_1=0.0372, wR_2 = 0.0992	R_1 = 0.0353, wR_2 = 0.0899	R_1 = 0.0485, wR_2 = 0.1471	R_1 = 0.0579, wR_2 = 0.1316
R indices R_1, wR_2 (all data)	$R1$ = 0.0501, wR_2 = 0.1049	R_1 = 0.0453, wR_2 = 0.0977	R_1 = 0.0584, wR_2 = 0.1559	R_1 = 0.1017, wR_2 = 0.1601

Largest diff. peak and hole / $e{\cdot}Å^{-3}$	0.258, -0.213	0.314, -0.355	0.489, -0.443	0.601, -0.666

	5	**6**	**7**
Formula	$C_7H_{22}Cl_2CoN_6NaO_{5.69}S$	$C_{14}H_{26}ClCoK_2N_6O_{10}S_2$	$C_{36}H_{46}CoN_{14}O_{14}S_2$
M_r/g mol^{-1}	466.18	675.11	1021.92
T/K	293(2)	293(2)	293(2)
Cryst. system	Monoclinic	Tetragonal	Triclinic
Space group	$P2_1/m$	$I4/m$	P-1
a/Å	14.489(3)	14.3265(5)	12.9654(5)
b/Å	6.8710(10)	14.3265(5)	13.1933(6)
c/Å	17.692(3)	24.7933(16)	16.5514(9)
α/°	90	90	83.432(4)
β/°	97.903(17)	90	72.016(4)
γ/°	90	90	68.761(4)
V/Å^3	1744.6(5)	5088.8(5)	2510.0(2)
Z	4	8	2
D_{calcd} / mg/m^3	1.775	1.762	1.352
μ / mm^{-1}	1.470	1.332	0.498
F(000)	958	2768	1062
Crystal size / mm^3	0.350x0.080x0.020	0.500x0.300x0.060	0.550x0.400x0.210
Theta range for data collection / °	3.185 – 25.242	3.284 – 25.467	3.0687 – 30.9703
Index ranges	-17≤ h ≤10, -8<=k<=8, -21<=l<=21	-10<=h<=17, -17<=k<=8, -27<=l<=30	-12<=h<=18, -16<=k<=18, -20<=l<=22
Refls collected/independent	3869/3869	6586/2428 (R_{int}=0.0439)	20488/9304 (R_{int}=0.0307)
Completeness to theta / % (θ = 25.50)	99.4	99.7	2822.05
Data/restrains/parameters	3869 / 36 / 274	2428 / 0 / 180	9304 / 22 / 645

Goodness-of-fit on F^2	1.009	1.007	1.001
Final R_1, wR_2	$R_1 = 0.0528$, $wR_2 = 0.0847$	$R_1 = 0.0435$, $wR_2 = 0.1095$	$R_1 = 0.0648$, $wR_2 = 0.1764$
R indices R_1, wR_2 (all data)	$R_1 = 0.1081$, $wR_2 = 0.0902$	$R_1 = 0.0621$, $wR_2 = 0.1200$	$R_1 = 0.1000$, $wR_2 = 0.2021$
Largest diff. peak and hole / $e{\cdot}Å^{-3}$	0.887, -0.804	0.767, -0.513	0.695, -0.358

Table S3. Selected bond distances (Å) and angles (°) in **1**–**7**

Bond	*d*, Å	Angle	ω, °	Angle	ω, °
1					
Co1–N1	1.958(3)	N(1)Co(1)N(1)$^{\#1}$	179.73(17)	N(1)$^{\#1}$Co(1)N(2)$^{\#3}$	89.86(8)
Co1–N1$^{\#1}$	1.958(3)	N(1)Co(1)N(1)$^{\#2}$	89.77(16)	N(1)$^{\#2}$Co(1)N(2)$^{\#3}$	90.14(8)
Co1–N1$^{\#2}$	1.958(3)	N(1)$^{\#1}$Co(1)N(1)$^{\#2}$	90.24(16)	N(1)$^{\#3}$Co(1)N(2)$^{\#3}$	90.14(8)
Co1–N1$^{\#3}$	1.958(3)	N(1)Co(1)N(1)$^{\#3}$	90.23(16)	N(1)Co(1)N(2)	90.14(8)
Co1–N2$^{\#3}$	1.968(4)	N(1)$^{\#1}$Co(1)N(1)$^{\#3}$	89.77(16)	N(1)$^{\#1}$Co(1)N(2)	90.14(8)
Co1–N2	1.968(4)	N(1)$^{\#2}$Co(1)N(1)$^{\#3}$	179.73(17)	N(1)$^{\#2}$Co(1)N(2)	89.86(8)
		N(1)Co(1)N(2)$^{\#3}$	89.86(8)	N(1)$^{\#3}$Co(1)N(2)	89.86(8)
2					
Co1–N3$^{\#1}$	1.962(2)	N(3)$^{\#1}$Co(1)N(3)	180.0	N(1)Co(1)N(2)$^{\#1}$	91.30(9)
Co1–N3	1.962(2)	N(3)$^{\#1}$Co(1)N(1)	88.43(9)	N(1)$^{\#1}$Co(1)N(2)$^{\#1}$	88.70(9)
Co1–N1	1.962(2)	N(3)Co(1)N(1)	91.57(9)	N(3)$^{\#1}$Co(1)N(2)	89.68(9)
Co1–N1$^{\#1}$	1.963(2)	N(3)$^{\#1}$Co(1)N(1)$^{\#1}$	91.57(9)	N(3)Co(1)N(2)	90.32(9)
Co1–N2$^{\#1}$	1.966(2)	N(3)Co(1)N(1)$^{\#1}$	88.43(9)	N(1)Co(1)N(2)	88.70(9)
Co1–N2	1.966(2)	N(1)Co(1)N(1)$^{\#1}$	180.0	N(1)$^{\#1}$Co(1)N(2)	91.30(9)
		N(3)$^{\#1}$Co(1)N(2)$^{\#1}$	90.32(9)	N(2)$^{\#1}$Co(1)N(2)	180.0
		N(3)Co(1)N(2)$^{\#1}$	89.68(9)		
3					
Co1–N1	1.948(4)	N(1)Co(1)N(4)	89.08(13)	N(4)$^{\#1}$Co(1)N(3)$^{\#1}$	90.96(13)

Co1–N4	1.951(3)	N(1)Co(1)N(4)$^{\#1}$	89.08(13)	N(3)Co(1)N(3)$^{\#1}$	88.19(17)
Co1–N4$^{\#1}$	1.951(3)	N(4)Co(1)N(4)$^{\#1}$	89.88(19)	N(1)Co(1)N(2)	179.26(17)
Co1–N3	1.962(3)	N(1)Co(1)N(3)	90.15(12)	N(4)Co(1)N(2)	90.40(13)
Co1–N3$^{\#1}$	1.962(3)	N(4)Co(1)N(3)	90.96(13)	N(4)$^{\#1}$Co(1)N(2)	90.40(13)
Co1–N2	1.979(4)	N(4)$^{\#1}$Co(1)N(3)	178.85(13)	N(3)Co(1)N(2)	90.38(13)
		N(1)Co(1)N(3)$^{\#1}$	90.15(12)	N(3)$^{\#1}$Co(1)N(2)	90.38(13)
		N(4)Co(1)N(3)$^{\#1}$	178.85(12)		
4					
Co1–N3$^{\#1}$	1.956(4)	N(3)$^{\#1}$Co(1)N(3)	180.0	N(4)Co(2)N(6)	90.75(19)
Co1–N3	1.956(4)	N(3)$^{\#1}$Co(1)N(2)$^{\#1}$	90.77(19)	N(5)Co(2)N(6)	91.2(2)
Co1–N2$^{\#1}$	1.962(5)	N(3)Co(1)N(2)$^{\#1}$	89.23(19)	N(9)Co(2)N(7)	90.0(2)
Co1–N2	1.962(5)	N(3)$^{\#1}$Co(1)N(2)	89.23(19)	N(8)Co(2)N(7)	89.6(2)
Co1–N1$^{\#1}$	1.962(4)	N(3)Co(1)N(2)	90.77(19)	N(4)Co(2)N(7)	178.0(2)
Co1–N1	1.962(4)	N(2)$^{\#1}$Co(1)N(2)	180.0	N(5)Co(2)N(7)	90.4(2)
Co2–N9	1.953(4)	N(3)$^{\#1}$Co(1)N(1)$^{\#1}$	90.00(18)	N(6)Co(2)N(7)	90.9(2)
Co2–N8	1.954(5)	N(3)Co(1)N(1)$^{\#1}$	90.00(18)	N(10)$^{\#2}$Co(3)N(10)	180.0
Co2–N4	1.960(4)	N(2)$^{\#1}$Co(1)N(1)$^{\#1}$	88.4(2)	N(10)$^{\#2}$Co(3)N(12)	90.2(2)
Co2–N5	1.964(5)	N(2)Co(1)N(1)$^{\#1}$	91.6(2)	N(10)Co(3)N(12)	89.8(2)
Co2–N6	1.965(5)	N(3)$^{\#1}$Co(1)N(1)	90.00(18)	N(10)$^{\#2}$Co(3)N(12)$^{\#2}$	89.8(2)
Co2–N7	1.966(4)	N(3)Co(1)N(1)	90.00(18)	N(10)Co(3)N(12)$^{\#2}$	90.2(2)
Co3–N10$^{\#2}$	1.953(5)	N(2)$^{\#1}$Co(1)N(1)	91.6(2)	N(12)Co(3)N(12)$^{\#2}$	180.0
Co3–N10	1.953(5)	N(2)Co(1)N(1)	88.4(2)	N(10)$^{\#2}$Co(3)N(11)	90.2(2)
Co3–N12	1.957(4)	N(1)$^{\#1}$Co(1)N(1)	180.0(3)	N(10)Co(3)N(11)	89.8(2)
Co3–N12$^{\#2}$	1.957(4)	N(9)Co(2)N(8)	88.9(2)	N(12)Co(3)N(11)	89.75(19)
Co3–N11	1.962(4)	N(9)Co(2)N(4)	88.38(19)	N(12)$^{\#2}$Co(3)N(11)	90.3(2)
Co3–N11$^{\#2}$	1.962(4)	N(8)Co(2)N(4)	91.6(2)	N(10)$^{\#2}$Co(3)N(11)$^{\#2}$	89.8(2)
		N(9)Co(2)N(5)	89.8(2)	N(10)Co(3)N(11)$^{\#2}$	90.2(2)
		N(8)Co(2)N(5)	178.7(2)	N(12)Co(3)N(11)$^{\#2}$	90.3(2)
		N(4)Co(2)N(5)	88.4(2)	N(12)$^{\#2}$Co(3)N(11)$^{\#2}$	89.75(19)
		N(9)Co(2)N(6)	178.65(19)	N(11)Co(3)N(11)$^{\#2}$	180.00(17)
		N(8)Co(2)N(6)	90.1(2)		
5					

Co1–N4	1.956(8)	N(4)Co(1)N(3)	87.6(3)	N(7)Co(2)N(6)	88.0(3)
Co1–N3	1.960(6)	N(4)Co(1)N(3)$^{\#1}$	87.6(3)	N(7)$^{\#2}$Co(2)N(6)	88.0(3)
Co1–N3$^{\#1}$	1.960(6)	N(3)Co(1)N(3)$^{\#1}$	90.4(4)	N(8)Co(2)N(6)	177.3(4)
Co1–N2	1.974(8)	N(4)Co(1)N(2)	176.7(4)	N(5)$^{\#2}$Co(2)N(6)	91.6(3)
Co1–N1$^{\#1}$	1.979(6)	N(3)Co(1)N(2)	90.0(3)	N(5)Co(2)N(6)	91.6(3)
Co1–N1	1.979(6)	N(3)$^{\#1}$Co(1)N(2)	90.0(3)	O(2)Na(1)O(3)$^{\#3}$	88.26(17)
Co2–N7	1.957(6)	N(4)Co(1)N(1)$^{\#1}$	91.2(3)	O(2)Na(1)O(3)$^{\#4}$	88.26(17)
Co2–N7$^{\#2}$	1.957(6)	N(3)Co(1)N(1)$^{\#1}$	178.8(3)	O(3)$^{\#3}$Na(1)O(3)$^{\#4}$	138.2(3)
Co2–N8	1.960(9)	N(3)$^{\#1}$Co(1)N(1)$^{\#1}$	89.3(2)	O(2)Na(1)Cl(1)	104.5(3)
Co2–N5$^{\#2}$	1.982(5)	N(2)Co(1)N(1)$^{\#1}$	91.2(3)	O(3)$^{\#3}$Na(1)Cl(1)	110.57(16)
Co2–N5	1.982(6)	N(4)Co(1)N(1)	91.2(3)	O(3)$^{\#4}$Na(1)Cl(1)	110.57(16)
Co2–N6	1.984(9)	N(3)Co(1)N(1)	89.3(2)	O(2)Na(1)Cl(2)	167.5(3)
Na1–O2	2.275(9)	N(3)$^{\#1}$Co(1)N(1)	178.8(3)	O(3)$^{\#3}$Na(1)Cl(2)	87.27(15)
Na1–O3$^{\#3}$	2.402(5)	N(2)Co(1)N(1)	91.2(3)	O(3)$^{\#4}$Na(1)Cl(2)	87.28(15)
Na1–O3$^{\#4}$	2.402(5)	N(1)$^{\#1}$Co(1)N(1)	91.0(3)	Cl(1)Na(1)Cl(2)	88.09(16)
Na1–Cl1	2.707(6)	N(7)Co(2)N(7)$^{\#2}$	92.4(4)	O(6)$^{\#5}$Na(2)O(6)	155.2(4)
Na1–Cl2	2.788(5)	N(7)Co(2)N(8)	90.1(3)	O(6)$^{\#5}$Na(2)O(7)$^{\#6}$	92.40(17)
Na2–O6$^{\#5}$	2.299(5)	N(7)$^{\#2}$Co(2)N(8)	90.1(3)	O(6)Na(2)O(7)$^{\#6}$	92.40(17)
Na2–O6	2.299(5)	N(7)Co(2)N(5)$^{\#2}$	178.5(3)	O(6)$^{\#5}$Na(2)Cl(4)	101.41(19)
Na2–O7$^{\#6}$	2.426(9)	N(7)$^{\#2}$Co(2)N(5)$^{\#2}$	88.9(3)	O(6)Na(2)Cl(4)	101.41(19)
Na2–Cl4	2.801(6)	N(8)Co(2)N(5)$^{\#2}$	90.3(3)	O(7)$^{\#6}$Na(2)Cl(4)	101.5(2)
Na2–Cl3	3.077(5)	N(7)Co(2)N(5)	88.9(3)	O(6)$^{\#5}$Na(2)Cl(3)	78.65(17)
		N(7)$^{\#2}$Co(2)N(5)	178.5(3)	O(6)Na(2)Cl(3)	78.65(17)
		N(8)Co(2)N(5)	90.3(3)	O(7)$^{\#6}$Na(2)Cl(3)	124.7(3)
		N(5)$^{\#2}$Co(2)N(5)	89.7(4)	Cl(4)Na(2)Cl(3)	133.73(18)
6					
Co1–N3$^{\#1}$	1.949(4)	N(3)$^{\#1}$Co(1)N(3)	180.0	N(7)Co(3)N(7)$^{\#5}$	180.0
Co1–N3	1.949(4)	N(3)$^{\#1}$Co(1)N(2)	91.5(2)	N(7)Co(3)N(7)$^{\#6}$	90.0
Co1–N2	1.958(4)	N(3)Co(1)N(2)	88.5(2)	N(7)$^{\#5}$Co(3)N(7)$^{\#6}$	90.000(1)
Co1–N2$^{\#1}$	1.958(4)	N(3)$^{\#1}$Co(1)N(2)$^{\#1}$	88.5(2)	N(7)Co(3)N(7)$^{\#4}$	90.001(1)
Co1–N1	1.960(4)	N(3)Co(1)N(2)$^{\#1}$	91.5(2)	N(7)$^{\#5}$Co(3)N(7)$^{\#4}$	90.0
Co1–N1$^{\#1}$	1.960(4)	N(2)Co(1)N(2)$^{\#1}$	180.0	N(7)$^{\#6}$Co(3)N(7)$^{\#4}$	180.0

Co2–N4	1.960(5)	N(3)$^{\#1}$Co(1)N(1)	90.000(1)	N(7)Co(3)N(6)$^{\#5}$	90.0
Co2–N4$^{\#2}$	1.960(5)	N(3)Co(1)N(1)	90.000(1)	N(7)$^{\#5}$Co(3)N(6)$^{\#5}$	90.0
Co2–N5	1.965(4)	N(2)Co(1)N(1)	90.0	N(7)$^{\#6}$Co(3)N(6)$^{\#5}$	90.0
Co2–N5$^{\#2}$	1.965(4)	N(2)$^{\#1}$Co(1)N(1)	90.0	N(7)$^{\#4}$Co(3)N(6)$^{\#5}$	90.0
Co2–N5$^{\#3}$	1.965(4)	N(3)$^{\#1}$Co(1)N(1)$^{\#1}$	90.000(1)	N(7)Co(3)N(6)	90.0
Co2–N5$^{\#4}$	1.965(4)	N(3)Co(1)N(1)$^{\#1}$	90.000(1)	N(7)$^{\#5}$Co(3)N(6)	90.0
Co3–N7	1.967(4)	N(2)Co(1)N(1)$^{\#1}$	90.0	N(7)$^{\#6}$Co(3)N(6)	90.0
Co3–N7$^{\#5}$	1.967(4)	N(2)$^{\#1}$Co(1)N(1)$^{\#1}$	90.0	N(7)$^{\#4}$Co(3)N(6)	90.0
Co3–N7$^{\#6}$	1.967(4)	N(1)Co(1)N(1)$^{\#1}$	180.0	N(6)$^{\#5}$Co(3)N(6)	180.0
Co3–N7$^{\#4}$	1.967(4)	N(4)Co(2)N(4)$^{\#2}$	180.0	O(2)$^{\#7}$K(1)O(4)	159.95(8)
Co3–N6$^{\#5}$	1.969(5)	N(4)Co(2)N(5)	90.000(2)	O(2)$^{\#7}$K(1)O(3)$^{\#4}$	73.52(7)
Co3–N6	1.969(5)	N(4)$^{\#2}$Co(2)N(5)	90.000(2)	O(4)K(1)O(3)$^{\#4}$	126.35(8)
K1–O2$^{\#7}$	2.708(3)	N(4)Co(2)N(5)$^{\#2}$	90.000(2)	O(2)$^{\#7}$K(1)O(1)$^{\#8}$	81.78(8)
K1–O4	2.716(3)	N(4)$^{\#2}$Co(2)N(5)$^{\#2}$	90.000(2)	O(4)K(1)O(1)$^{\#8}$	78.29(8)
K1–O3$^{\#4}$	2.776(3)	N(5)Co(2)N(5)$^{\#2}$	180.0	O(3)$^{\#4}$K(1)O(1)$^{\#8}$	155.27(8)
K1–O1$^{\#8}$	2.787(3)	N(4)Co(2)N(5)$^{\#3}$	90.000(1)	O(2)$^{\#7}$K(1)O(5)$^{\#4}$	122.61(8)
K1–O5$^{\#4}$	2.933(3)	N(4)$^{\#2}$Co(2)N(5)$^{\#3}$	90.000(1)	O(4)K(1)O(5)$^{\#4}$	76.82(8)
K1–Cl1	2.9614(11)	N(5)Co(2)N(5)$^{\#3}$	90.000(2)	O(3)$^{\#4}$K(1)O(5)$^{\#4}$	49.73(7)
		N(5)$^{\#2}$Co(2)N(5)$^{\#3}$	90.000(1)	O(1)$^{\#8}$K(1)O(5)$^{\#4}$	154.12(8)
		N(4)Co(2)N(5)$^{\#4}$	90.000(1)	O(2)$^{\#7}$K(1)Cl(1)	91.59(7)
		N(4)$^{\#2}$Co(2)N(5)$^{\#4}$	90.000(1)	O(4)K(1)Cl(1)	87.91(7)
		N(5)Co(2)N(5)$^{\#4}$	90.000(1)	O(3)$^{\#4}$K(1)Cl(1)	85.19(6)
		N(5)$^{\#2}$Co(2)N(5)$^{\#4}$	90.000(2)	O(1)$^{\#8}$K(1)Cl(1)	94.63(7)
		N(5)$^{\#3}$Co(2)N(5)$^{\#4}$	180.0	O(5)$^{\#4}$K(1)Cl(1)	77.55(6)
7					
Co1–N1	1.944(3)	N(1)Co(1)N(2)	88.05(14)	N(6)Co(1)N(4)	91.24(15)
Co1–N2	1.948(3)	N(1)Co(1)N(6)	87.40(15)	N(3)Co(1)N(4)	89.41(13)
Co1–N3	1.959(3)	N(2)Co(1)N(6)	91.54(15)	N(1)Co(1)N(5)	90.02(16)
Co1–N4	1.961(3)	N(1)Co(1)N(3)	91.97(13)	N(2)Co(1)N(5)	176.23(16)
Co1–N5	1.963(4)	N(2)Co(1)N(3)	89.30(14)	N(6)Co(1)N(5)	91.60(17)
Co1–N6	1.959(3)	N(6)Co(1)N(3)	178.93(16)	N(3)Co(1)N(5)	87.53(16)
		N(1)Co(1)N(4)	177.98(16)	N(4)Co(1)N(5)	91.52(17)

	N(2)Co(1)N(4)	90.49(15)

Symmetry transformations used to generate equivalent atoms:
1: #1 -*x*+1/4,-*y*+5/4,*z* #2 -*x*+1/4,*y*,-*z*+5/4 #3 *x*,-*y*+5/4,-*z*+5/4
2: #1 -*x*+1,-*y*,-*z*+1
3: #1 -*x*,-*y*+1,-*z*+2 #2 -*x*+1,-*y*+1,-*z*+2 #3 *y*,-*x*+1,-*z*+2 #4 -*y*+1,*x*,*z* #5 -*x*+1,-*y*+1,-*z*+1 #6 *y*,-*x*+1,-*z*+1
4: #1 *x*,-*y*+3/2,*z*
5: #1 -*x*+2,-*y*+1,-*z*+2 #2 -*x*+1,-*y*+2,-*z* #3 -*x*+1,*y*-1/2,-*z*+1 #4 -*x*+1,-*y*+1,-*z*+1 #5 *x*,-*y*+5/2,*z* #6 -*x*+2,-*y*+2,-*z*+2
6: #1 *x*,-*y*+1/2,*z* #2 *x*,-*y*+3/2,*z* #3 *y*,-*x*+1,-*z*+2 #4 -*y*+1,*x*,*z* #5 -*x*+1,-*y*+1,-*z*+1 #6 *y*,-*x*+1,-*z*+1 #7 -*x*+1/2,-*y*+1/2,-*z*+3/2 #8 *y*-1/2,-*x*+1/2,-*z*+3/2
#9 *y*,-*x*+1,*z* #10 *x*,*y*,-*z*+1 #11 -*y*+1/2,*x*+1/2,-*z*+3/2

Table S4. Details of the hydrogen bonding interactions in **1**-**7**

Contact D–H···A	Distance, Å			Angle	Symmetry
	D···H	H···A	D···A	DHA, °	transformations
1					
N1–H1A...O1	0.89	2.12	2.977(4)	162.2	*x*-1/2,*y*+1/2,*z*
N1–H1B...O2	0.89	2.15	2.951(4)	149.5	-*x*+1,-*y*+1,-*z*+1
N1–H1B...O2	0.89	2.62	3.058(4)	111.7	-*x*+1,*y*+1/4,*z*+1/4
N1–H1C...O3	0.89	2.22	3.056(4)	157.4	-*x*+3/4,*y*+1/2,-*z*+5/4
N2–H2A...O3	0.89	2.35	3.120(4)	145.2	-*x*+3/4,*y*+1/2,-*z*+5/4
N2–H2B...O1	0.89	2.43	3.269(4)	157.6	-*x*+1,*y*+1/4,*z*+1/4
N2–H2B...O2	0.89	2.66	3.387(3)	140.1	-*x*+1,*y*+1/4,*z*+1/4
N2–H2C...O3	0.89	2.44	3.120(4)	133.6	*x*-1/2,-*y*+3/4,-*z*+5/4
C4–H4...N3	0.93	2.34	2.958(14)	124.0	-*x*+3/4,-*y*+3/4,*z*
C6–H6B...O3	0.93	2.36	3.209(11)	151.7	*x*+1/4,*y*+1/4,-*z*+1
C13–H13...O2	0.93	2.62	3.52(3)	164.0	-*x*+1,*y*+1/4,*z*+1/4
N9–H6A...N9	0.82	2.03	2.82(2)	167.2	-*x*+5/4,-*y*+5/4,*z*
2					
N1–H1A...Cl1	0.89	2.50	3.366(2)	164.8	
N1–H1B...O2	0.89	2.13	3.023(3)	176.5	
N1–H1C...O3	0.89	2.11	2.994(3)	174.4	*x*+1,*y*,*z*
N2–H2A...O2	0.89	2.41	3.214(3)	150.4	-*x*+1,-*y*+2,-*z*+1
N2–H2B...Cl1	0.89	2.51	3.360(2)	159.7	
N2–H2C...O1	0.89	2.13	3.013(3)	168.9	*x*+1,*y*,*z*
N3–H3A...O1	0.89	2.15	3.027(3)	168.1	-*x*+1,-*y*+2,-*z*+1
N3–H3B...O3	0.89	2.53	3.315(3)	147.8	*x*+1,*y*,*z*
N3–H3B...N5	0.89	2.63	3.155(4)	119.0	*x*,*y*+1,*z*
N3–H3C...Cl1	0.89	2.56	3.411(2)	160.0	*x*,*y*+1,*z*
C3–H3...O2	0.93	3.46	3.467(4)	152.4	*x*,*y*-1,*z*
3					
N1–H1Aa...O1	0.89	2.14	2.997(4)	160.3	-*x*+1,*y*+1/2,-*z*+1
N1–H1Ba...O1	0.89	2.27	2.997(4)	139.2	-*x*+1,-*y*+1,-*z*+1
N1–H1Ba...Cl1	0.89	2.81	3.422(4)	127.4	*x*-1/2,*y*,-*z*+1/2
N1–H1Ca...O3	0.89	2.09	2.864(6)	145.2	*x*,*y*,*z*-1
N2–H2Aa...Cl1	0.89	2.80	3.643(5)	159.6	-*x*+1,-*y*+2,-*z*+1
N2–H2Ca...O1	0.89	2.36	3.233(5)	166.9	*x*-1/2,*y*,-*z*+3/2
N3–H3A...Cl1	0.89	2.57	3.430(3)	163.0	*x*-1/2,*y*,-*z*+1/2
N3–H3B...O1	0.89	2.20	3.088(4)	176.3	*x*-1/2,*y*,-*z*+3/2
N3–H3C...O2	0.89	2.40	3.183(4)	147.2	-*x*+1,-*y*+1,-*z*+1
N3–H3C...Cl1	0.89	2.94	3.433(3)	116.3	-*x*+1,-*y*+1,-*z*+1
N4–H4A...O3	0.89	2.10	2.919(5)	152.4	*x*,*y*,*z*-1
N4–H4B...O2	0.89	2.17	3.040(4)	164.3	-*x*+1,-*y*+1,-*z*+1
N4–H4C...O6a	0.89	2.20	3.087(9)	177.4	
N4–H4C...O7b	0.89	2.09	2.875(9)	147.0	
O5–H5W...O6a	0.83	1.98	2.790(10)	165.7	
O5–H5W...O7b	0.83	2.34	3.036(11)	142.2	
4					
N1–H1A...O9	0.89	2.09	2.967(5)	168.6	
N1–H1B...O7	0.89	2.25	3.046(8)	149.2	-*x*+1,-*y*+1,-*z*+2
N1–H1B...Cl1	0.89	2.91	3.404(4)	116.3	-*x*+2,-*y*+1,-*z*+2
N1–H1C...Cl2	0.89	2.54	3.377(5)	156.7	-*x*+2,-*y*+1,-*z*+2

N2–H2A...O7	0.89	2.02	2.902(6)	169.6	*x*+1,*y*,*z*
N2–H2B...O8	0.89	2.05	2.940(6)	173.9	
N2–H2C...Cl2	0.89	2.47	3.333(5)	164.5	-*x*+2,-*y*+1,-*z*+2
N3–H3A...O8	0.89	2.19	3.055(7)	164.5	
N3–H3B...Cl2	0.89	2.59	3.347(5)	142.9	
N3–H3C...O9	0.89	2.07	2.956(7)	174.7	-*x*+1,-*y*+1,-*z*+2
N4–H4C...O4	0.89	2.17	3.039(5)	164.4	*x*-1,*y*,*z*
N4–H4A...O7	0.89	2.04	2.896(6)	159.8	
N4–H4B...O1	0.89	2.21	3.019(7)	150.7	-*x*+1,-*y*,-*z*+1
N5–H5A...O3	0.89	2.23	3.014(5)	146.6	*x*-1,*y*,*z*
N5–H5B...O1	0.89	2.04	2.887(7)	157.7	-*x*+1,-*y*,-*z*+1
N5–H5C...O5	0.89	2.13	3.003(6)	167.6	
N6–H6A...O3	0.89	2.55	3.178(6)	128.2	-*x*+1,-*y*+1,-*z*+1
N6–H6A...O4	0.89	2.52	3.129(6)	125.8	*x*-1,*y*,*z*
N6–H6C...Cl1	0.89	2.69	3.557(5)	163.9	*x*-1,*y*,*z*
N7–H7A...O5	0.89	2.58	3.410(7)	156.2	
N7–H7B...Cl1	0.89	2.57	3.427(5)	161.6	
N7–H7C...O12	0.89	2.14	2.966(7)	153.2	
N8–H8A...O7W	0.89	2.21	3.089(8)	170.8	
N8–H8B...Cl1	0.89	2.57	3.407(5)	155.9	
N8–H8C...O7	0.89	2.50	3.334(7)	156.0	
N8–H8C...O8	0.89	2.34	3.070(7)	139.9	
N9–H9A...O1	0.89	2.10	2.933(6)	154.8	-*x*+1,-*y*,-*z*+1
N9–H9B...O8	0.89	2.14	3.026(6)	170.7	
N9–H9C...O4	0.89	2.30	3.101(6)	149.7	
N9–H9C...Cl1	0.89	2.91	3.445(5)	120.2	
N10–H10A...O7W	0.89	2.40	3.127(7)	138.6	*x*,*y*,*z*-1
N10–H10B...O9	0.89	2.21	3.045(7)	156.2	-*x*+1,-*y*+1,-*z*+1
N10–H10C...O14	0.89	2.23	3.1(3)	154.3	*x*,*y*,*z*-1
N11–H11A...Cl2	0.89	2.86	3.346(5)	116.2	*x*-1,*y*,*z*-1
N11–H11B...Cl2	0.89	2.79	3.646(5)	161.5	-*x*+1,-*y*+2,-*z*+1
N11–H11C...O14	0.89	2.65	3.07(7)	110.4	-*x*+1,-*y*+2,-*z*+1
N12–H12A...O6	0.89	2.09	2.961(7)	164.5	-*x*+1,-*y*+1,-*z*+1
N12–H12A...O16a	0.89	2.65	3.14(2)	115.8	-*x*+1,-*y*+1,-*z*+1
N12–H12B...Cl2	0.89	2.87	3.377(5)	117.9	-*x*+2,-*y*+2,-*z*+1
N12–H12C...Cl2	0.89	2.48	3.359(6)	167.5	*x*,*y*,*z*-1
O11–H11W...O3	0.63(11)	2.27(11)	2.857(8)	156(14)	-*x*+2,-*y*+1,-*z*+1
O11–H12W...O13	1.00(9)	1.80(9)	2.797(11)	170(8)	*x*+1,*y*,*z*
O15b–H19Wb...O6	0.82(2)	2.46(14)	3.177(19)	145(21)	-*x*+1,-*y*,-*z*+1
O15b–H19Wb...O7	0.82(2)	2.53(13)	3.238(16)	145(20)	-*x*+1,-*y*+1,-*z*+1
O15b–H20Wb...O10	0.82(2)	2.1(2)	2.672(16)	126(24)	*x*-1,*y*,*z*
5					
N1–H1A...O8	0.89	2.15	3.034(9)	175.3	-*x*+1,-*y*+1,-*z*+1
N1–H1B...Cl3	0.89	2.47	3.323(7)	159.8	-*x*+1,-*y*+2,-*z*+1
N1–H1C...Cl1	0.89	2.78	3.565(6)	147.2	-*x*,-*y*+1,-*z*+1
N2–H2Ca...Cl1	0.89	2.50	3.295(9)	149.4	
N2–H2Aa...Cl1	0.89	2.62	3.4727(13)	161.2	-*x*,-*y*,-*z*+1
N3–H3C...Cl3	0.89	2.56	3.373(6)	152.4	-*x*+1,-*y*+2,-*z*+1
N3–H3A...O2	0.89	2.14	2.984(9)	157.8	
N3–H3B...Cl1	0.89	2.58	3.425(7)	159.4	-*x*,-*y*+1,-*z*+1
N4–H4Aa...O1	0.89	1.98	2.860(11)	170.4	
N4–H4Ba...Cl3	0.89	2.67	3.4545(10)	147.6	-*x*+1,-*y*+2,-*z*+1

N4–H4Ba...O6	0.89	2.62	3.222(8)	125.8	-*x*+1,*y*-1/2,-*z*+1
N4–H4Ca...Cl3	0.89	2.79	3.4545(9)	132.9	-*x*+1,-*y*+1,-*z*+1
N4–H4Ca...O6	0.89	2.58	3.222(8)	130.1	-*x*+1,-*y*+1,-*z*+1
N5–H5A...O3	0.89	2.14	3.015(8)	167.1	-*x*+1,*y*+1/2,-*z*+1
N5–H5B...O9d	0.89	2.13	2.915(19)	146.2	-*x*+1,-*y*+1,-*z*+1
N5–H5B...O10c	0.89	1.77	2.64(2)	163.3	-*x*+1,*y*+1/2,-*z*+1
N5–H5C...Cl2	0.89	2.95	3.505(7)	121.8	*x*,*y*+1,*z*
N5–H5C...Cl4	0.89	2.85	3.406(7)	122.0	
N6–H6Ca...O8	0.89	2.14	2.882(12)	140.8	*x*-1,*y*,*z*
N6–H6Ba...O3	0.89	2.22	3.087(9)	165.9	-*x*+1,-*y*+1,-*z*+1
N6–H6Ba...O3	0.89	2.63	3.087(9)	112.8	-*x*+1,*y*+1/2,-*z*+1
N6–H6Aa...Cl2	0.89	2.60	3.4624(13)	163.5	*x*,*y*+1,*z*
N7–H7B...Cl2	0.89	2.50	3.371(7)	168.0	*x*,*y*+1,*z*
N7–H7C...Cl4	0.89	2.84	3.560(7)	139.4	
N7–H7A...O7	0.89	2.08	2.957(9)	168.8	*x*-1,*y*,*z*
N8–H8Ba...Cl4	0.89	2.59	3.329(9)	140.8	-*x*+1,-*y*+2,-*z*+2
N8–H8Aa...Cl4	0.89	2.62	3.4791(17)	163.4	
6					
N1–H1A...O3	0.89	2.47	3.012(3)	119.3	-*y*+1/2,*x*+1/2,-*z*+3/2
N1–H1A...O4	0.89	2.39	3.272(3)	173.3	-*y*+1/2,*x*+1/2,-*z*+3/2
N1–H1B...O1	0.89	2.33	3.183(3)	159.6	-*x*,-*y*+1,*z*
N1–H1C...O3	0.89	2.15	3.012(3)	164.2	*y*-1/2,-*x*+1/2,-*z*+3/2
N2–H2A...O1	0.89	2.12	2.962(4)	157.7	*x*,*y*,-*z*+2
N2–H2B...O1	0.89	2.09	2.962(4)	167.9	
N2–H2C...Cl1	0.89	2.55	3.323(5)	145.6	-*x*+1/2,-*y*+1/2,-*z*+3/2
N3–H3A...Cl1	0.89	2.98	3.423(4)	113.0	-*y*+1/2,*x*+1/2,*z*+1/2
N3–H3A...O1	0.89	2.64	3.377(5)	140.3	
N3–H3B...O4	0.89	2.23	3.115(3)	175.9	-*y*+1/2,*x*+1/2,*z*+1/2
N3–H3C...O4	0.89	2.42	3.115(3)	135.6	-*y*+1/2,*x*+1/2,-*z*+3/2
N4–H4A...O2	0.89	2.08	2.948(3)	164.6	-*x*+1,-*y*+1,*z*
N4–H4B...O2	0.89	2.49	2.948(3)	112.2	
N4–H4B...O2	0.89	2.30	2.948(3)	130.0	*y*,-*x*+1,*z*
N4–H4C...O2	0.89	2.16	2.948(3)	146.9	-*y*+1,*x*,*z*
N5–H5A...O1	0.89	2.65	3.369(4)	139.1	*y*,-*x*+1,-*z*+2
N5–H5B...O2	0.89	2.17	2.982(3)	151.7	-*x*+1,-*y*+1,*z*
N5–H5C...O2	0.89	2.16	2.982(3)	153.4	-*x*+1,-*y*+1,-*z*+2
N6–H6A...O5	0.89	2.40	2.952(3)	120.2	-*x*+1,-*y*+1,*z*
N6–H6A...O5	0.89	2.33	2.952(3)	126.7	*y*,-*x*+1,*z*
N6–H6B...O5	0.89	2.12	2.952(3)	156.0	-*y*+1,*x*,*z*
N6–H6C...O5	0.89	2.09	2.952(3)	163.5	
N7–H7A...O5	0.89	2.50	3.345(3)	159.4	*x*,*y*,-*z*+1
N7–H7B...Cl1	0.89	2.68	3.323(4)	130.1	*y*,-*x*+1,-*z*+1
N7–H7B...O5	0.89	2.61	3.345(3)	140.8	
N7–H7C...Cl1	0.89	2.48	3.305(4)	155.2	
7					
O1–H18...O2	0.82	1.77	2.501(4)	147.3	
O6–H31...O7	0.82	1.78	2.507(4)	147.5	
N1–H1C...O4	0.89	2.13	2.982(5)	160.4	-*x*+1,-*y*+1,-*z*+1
N1–H1A...O2	0.89	2.16	3.031(5)	167.7	*x*,*y*,*z*-1
N1–H1B...O5	0.89	2.02	2.845(4)	152.9	
N2–H2A...O15	0.89	2.18	2.981(17)	148.7	*x*-1,*y*,*z*
N2–H2A...O17	0.89	2.38	3.15(2)	145.3	*x*-1,*y*,*z*

N2–H2A...O18	0.89	2.31	3.10(2)	147.3	*x*-1,*y*,*z*
N2–H2A...O22	0.89	2.42	3.08(2)	131.7	*x*-1,*y*,*z*
N2–H2B...O2	0.89	2.18	2.923(4)	140.9	*x*,*y*,*z*-1
N2–H2C...N8	0.89	2.22	3.113(5)	176.0	
N3–H3B...O5	0.89	2.18	2.981(4)	149.3	
N3–H3A...O10	0.89	2.36	3.132(4)	144.5	-*x*,-*y*+1,-*z*+1
N3–H3C...O7	0.89	2.23	3.087(4)	162.5	*x*-1,*y*+1,*z*+1
N4–H4B...O13	0.89	2.46	3.060(12)	125.4	*x*-1,*y*,*z*
N4–H4B...O14	0.89	2.44	3.195(13)	143.4	*x*-1,*y*,*z*
N4–H4B...O17	0.89	2.55	2.99(2)	110.8	*x*-1,*y*,*z*
N4–H4B...O19	0.89	2.25	2.98(3)	138.1	*x*-1,*y*,*z*
N4–H4B...O21	0.89	2.22	3.07(4)	160.5	*x*-1,*y*,*z*
N4–H4A...O8	0.89	2.20	3.058(6)	162.0	*x*-1,*y*+1,*z*+1
N4–H4C...O10	0.89	2.15	3.009(4)	160.6	-*x*,-*y*+1,-*z*+1
N5–H5C...O11	0.89	2.13	2.973(6)	157.6	-*x*+1,-*y*+1,-*z*+1
N5–H5A...O1	0.89	2.45	3.270(6)	153.4	-*x*+1,-*y*+1,-*z*+2
N5–H5B...O7	0.89	2.18	3.014(5)	156.6	*x*-1,*y*+1,*z*+1
N6–H6A...O11	0.89	2.17	2.989(7)	153.1	-*x*+1,-*y*+1,-*z*+1
N6–H6B...O13	0.89	2.38	3.103(12)	138.2	*x*-1,*y*,*z*
N6–H6B...O14	0.89	2.10	2.930(12)	155.8	*x*-1,*y*,*z*
N6–H6B...O21	0.89	2.48	3.27(3)	148.1	*x*-1,*y*,*z*
N6–H6C...O3	0.89	2.13	2.999(5)	165.3	*x*,*y*,*z*-1
N11–H11...O9	0.86	2.55	3.135(4)	126.1	-*x*,-*y*+1,-*z*
N11–H11...N12	0.86	2.14	2.993(5)	169.3	-*x*,-*y*+1,-*z*
O11–H33...O8	0.85	1.95	2.657(6)	140.0	*x*,*y*,*z*+1
O11–H34...O4	0.85	2.46	3.053(5)	127(4)	
O11–H34...O12	0.85	2.095	2.770(8)	136.1(6)	
O12–H36...N7	0.89	1.98	2.844(8)	166.6	
O12–H35...N14	0.85	2.594	3.420(8)	164.4(9)	*x*,*y*,*z*+1

Table S5. SAPT decomposition of the interaction energies (kcal/mol) for all found pairs in **1**-**7**[*]

Selected pairs		O…H, Å	E_{elst}	E_{exch}	E_{ind}	E_{disp}	E_{int}	d, Å
$[Co(NH_3)_6]^{3+} \cdot (pys)^-$ (**1**)	a	2.38 2.16	–220.024	11.956	–27.203	–4.913	–240.183	2.27
	b	2.19 2.18 2.14	–220.025	11.955	–27.193	–4.910	–240.173	2.17
	c	2.26 2.18 2.14	–219.496	11.409	–26.524	–4.821	–239.433	2.19
$[Co(NH_3)_6]^{3+} \cdot (pys)^-$ (**2**)	a	2.53 2.14 2.11	–221.330	11.686	–26.865	–4.762	–241.271	2.26
	b	2.41 2.15 2.13	–221.058	11.760	–26.877	–4.879	–241.054	2.23
$[Co(NH_3)_6]^{3+} \cdot (3\text{-sb})^{2-}$ (**3**)	a	2.40 2.17 2.15	–335.014	12.308	–32.273	–4.995	–359.974	2.24
	b	2.40 2.26 2.17	–334.066	11.142	–30.968	–4.806	–358.698	2.27
	c	2.37 2.20 2.20	–350.719	10.971	–30.926	–4.584	–375.258	2.25
	d	2.10 2.10 2.09	–330.671	17.774	–36.515	–5.375	–354.788	2.09
$[Co(NH_3)_6]^{3+} \cdot (3\text{-sb})^{2-}$ (**4**)	a	2.04 2.10	–326.317	15.753	–34.921	–4.952	–350.437	2.11

		2.20						
	b	2.60 2.23 2.18	–328.566	10.955	–30.759	–4.759	–353.129	2.33
	c	2.57 2.30 2.13	–342.426	11.859	–32.043	–5.342	–367.952	2.33
$[Co(NH_3)_6]^{3+} \cdot (3\text{-sbNa})^{-}$ (**5**)	a	2.08 2.08 2.14	–231.629	12.898	–33.541	–4.933	–257.205	2.10
$[Co(NH_3)_6]^{3+} \cdot (4\text{-sbK})^{-}$ (**6**)	a	2.64 2.16 2.08	–172.445	23.402	–159.255	–9.735	–318.033	2.29
	b	2.49 2.40	–130.462	6.424	–242.013	–2.590	–368.641	2.44
	c	2.64 2.30 2.16	–162.161	22.260	–154.438	–9.470	–303.809	2.37
$[Co(NH_3)_6]^{3+} \cdot (ssz)^{2-}$ (**7**)	a	2.23 2.18 2.02	–298.232	18.572	–45.901	–7.170	–332.731	2.14
	b	2.70 2.23 2.20 2.18	–302.705	16.557	–35.011	–5.213	–326.373	2.32
	c	2.18 2.16 2.13	–302.701	16.565	–35.018	–5.215	–326.368	2.15

*d - mean values of O…H hydrogen bonds

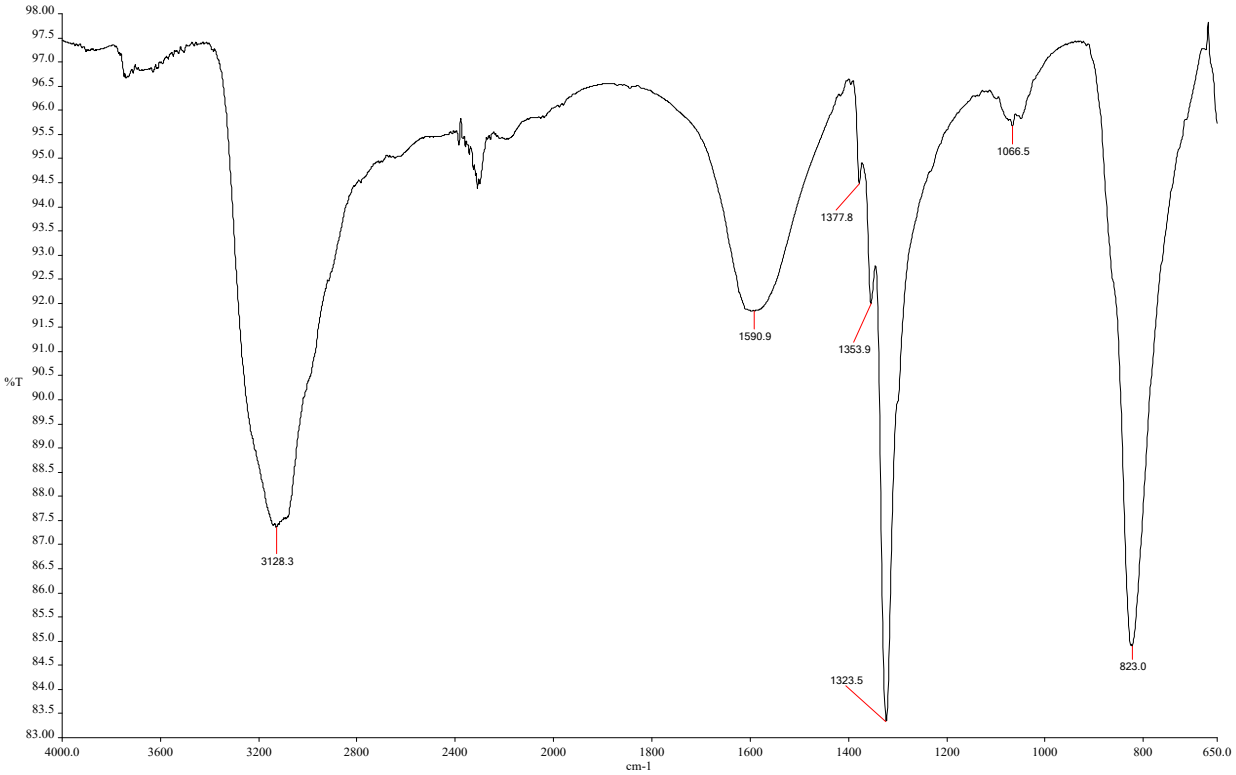


Fig. S1. IR spectrum of $[Co(NH_3)_6]Cl_3$.

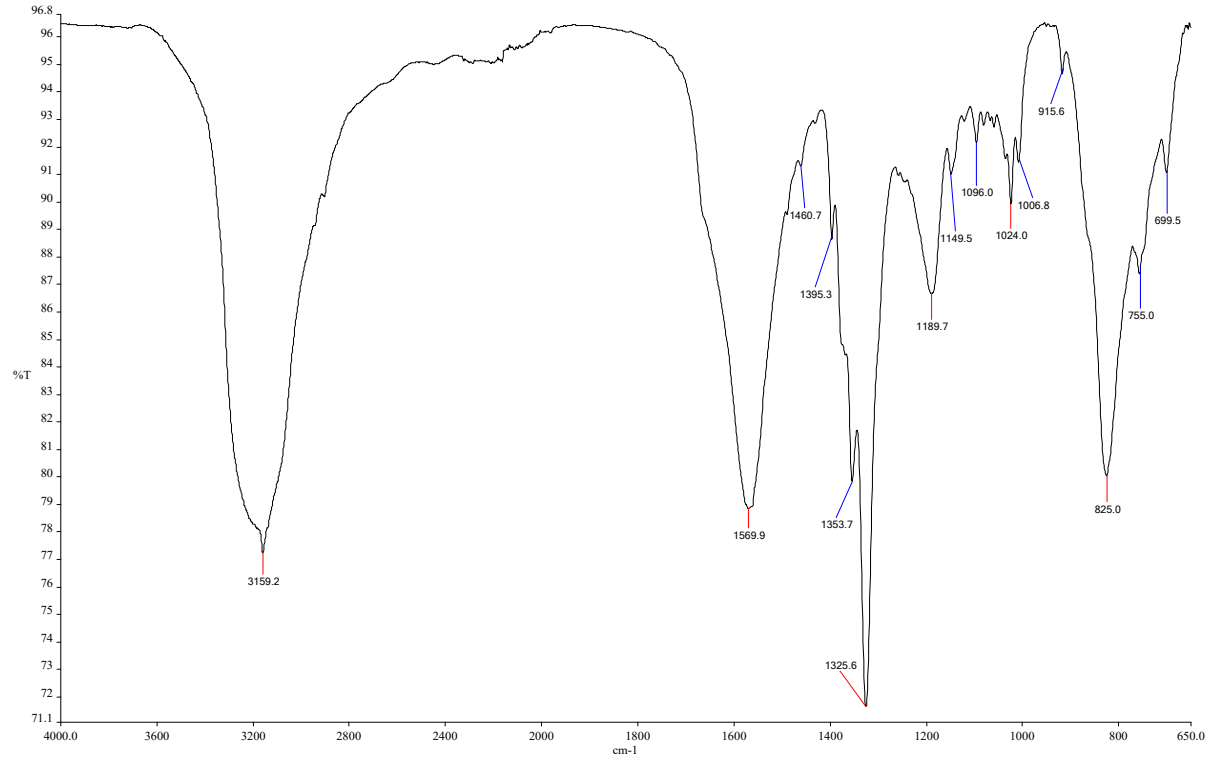


Fig. S2. IR spectrum of $[Co(NH_3)_6](pys)_3 \cdot Hpys$ (**1**).

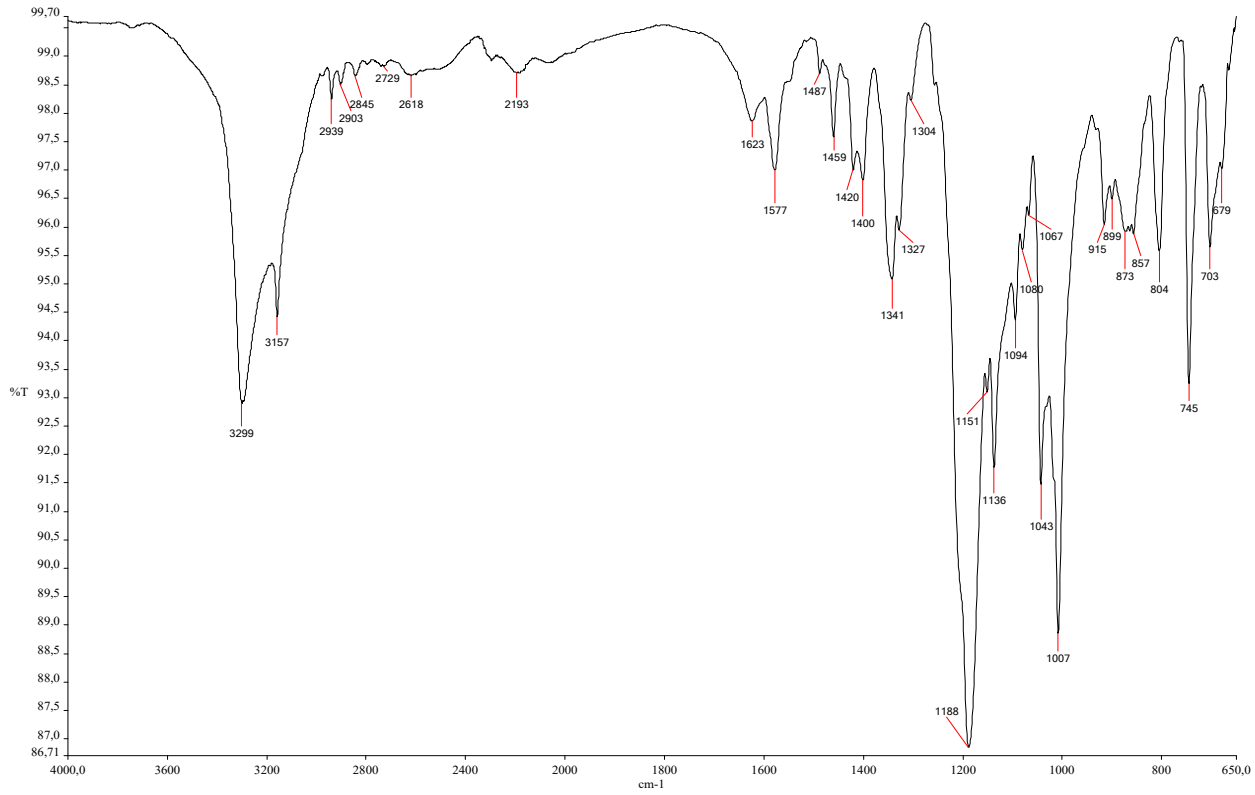


Fig. S3. IR spectrum of $[Co(NH_3)_6](pys)_2Cl \cdot 2MeCN$ (**2**).

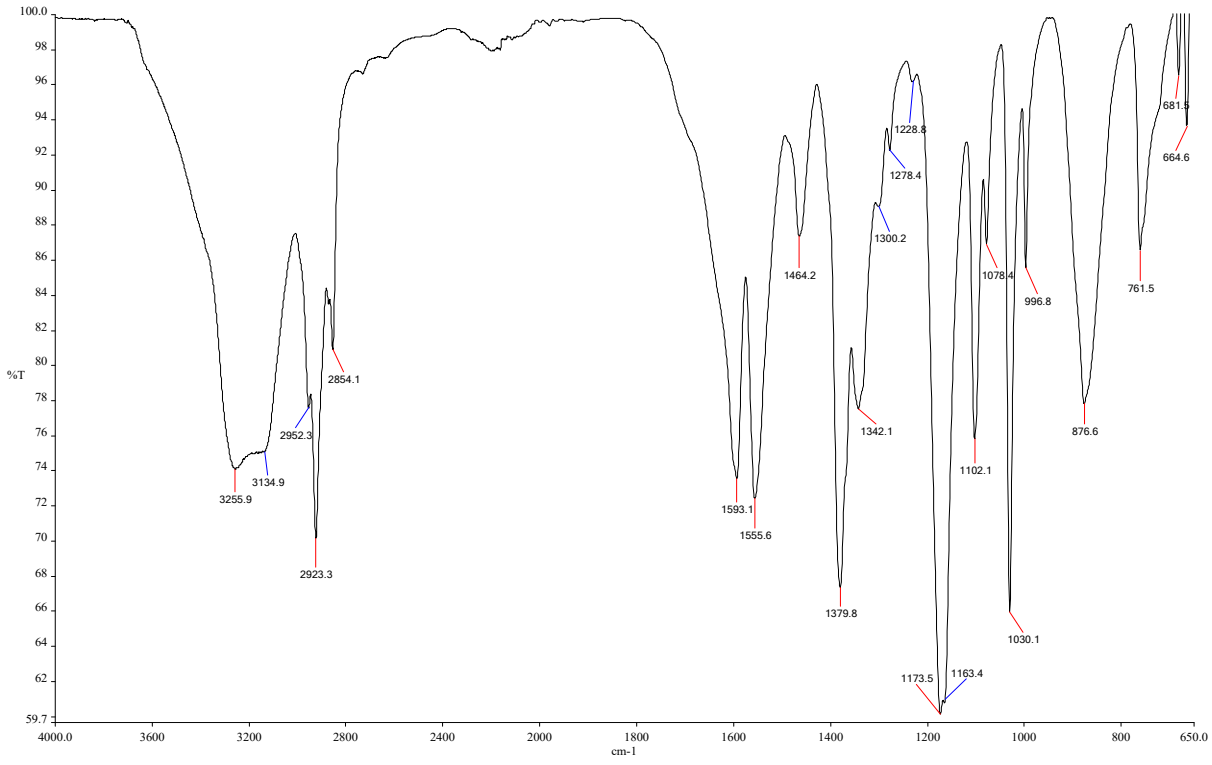


Fig. S4. IR spectrum of $[Co(NH_3)_6](3\text{-sb})Cl \cdot 4H_2O$ (**3**).

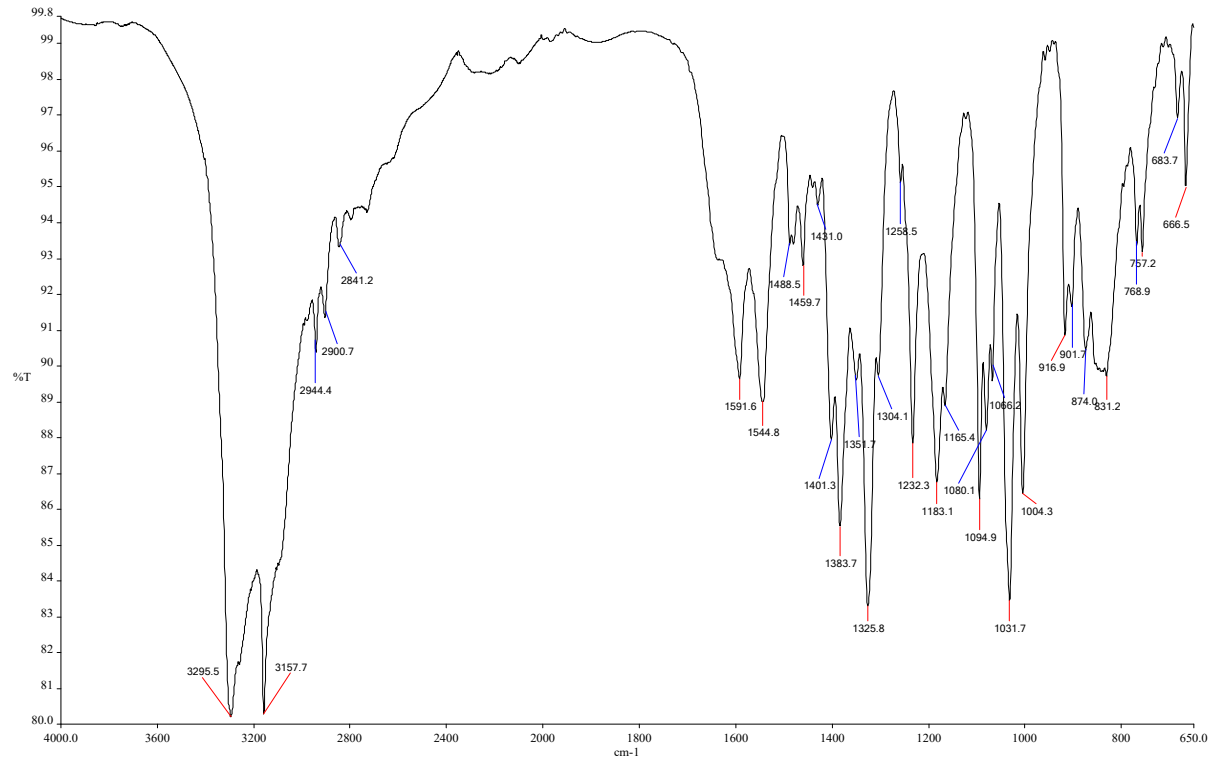


Fig. S5. IR spectrum of $[Co(NH_3)_6](3\text{-sb})(SO_4)Cl_2 \cdot 7H_2O$ (**4**).

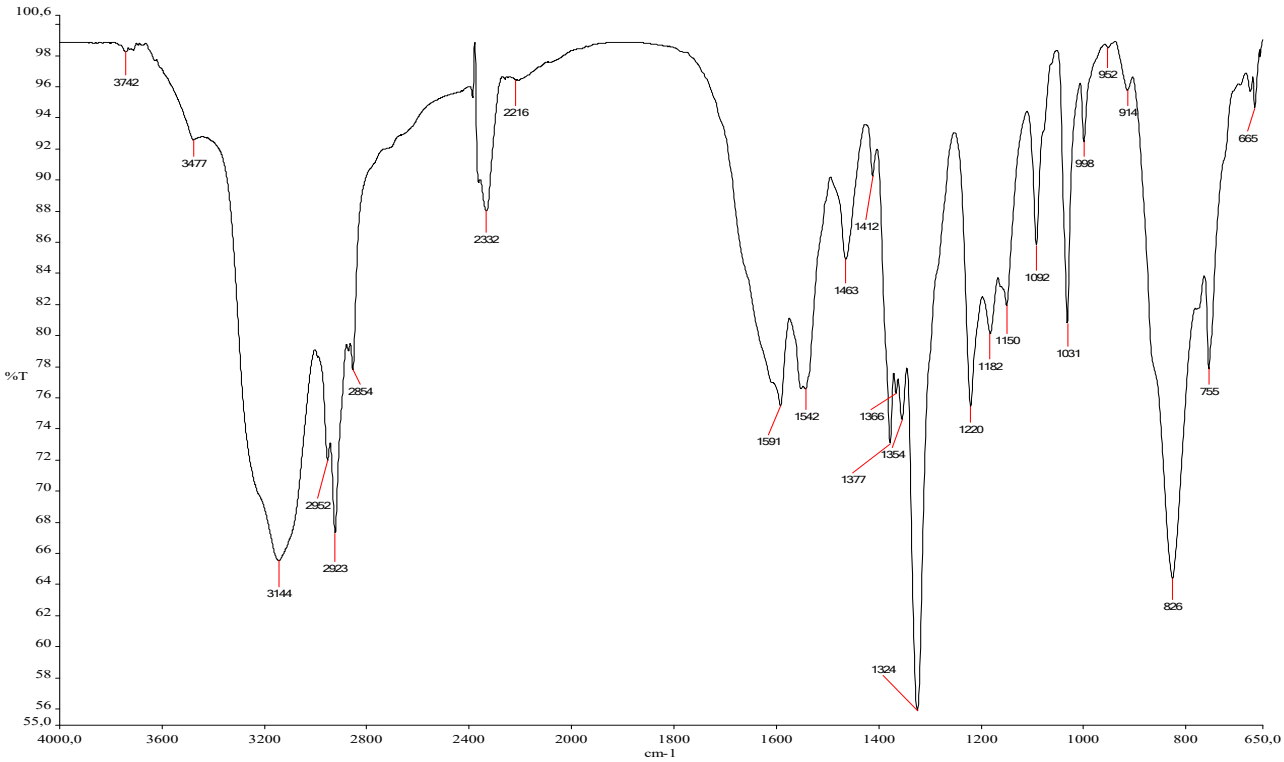


Fig. S6. IR spectrum of $\{[Co(NH_3)_6][Na(3\text{-sb})Cl_2] \cdot H_2O\}_n$ (**5**).

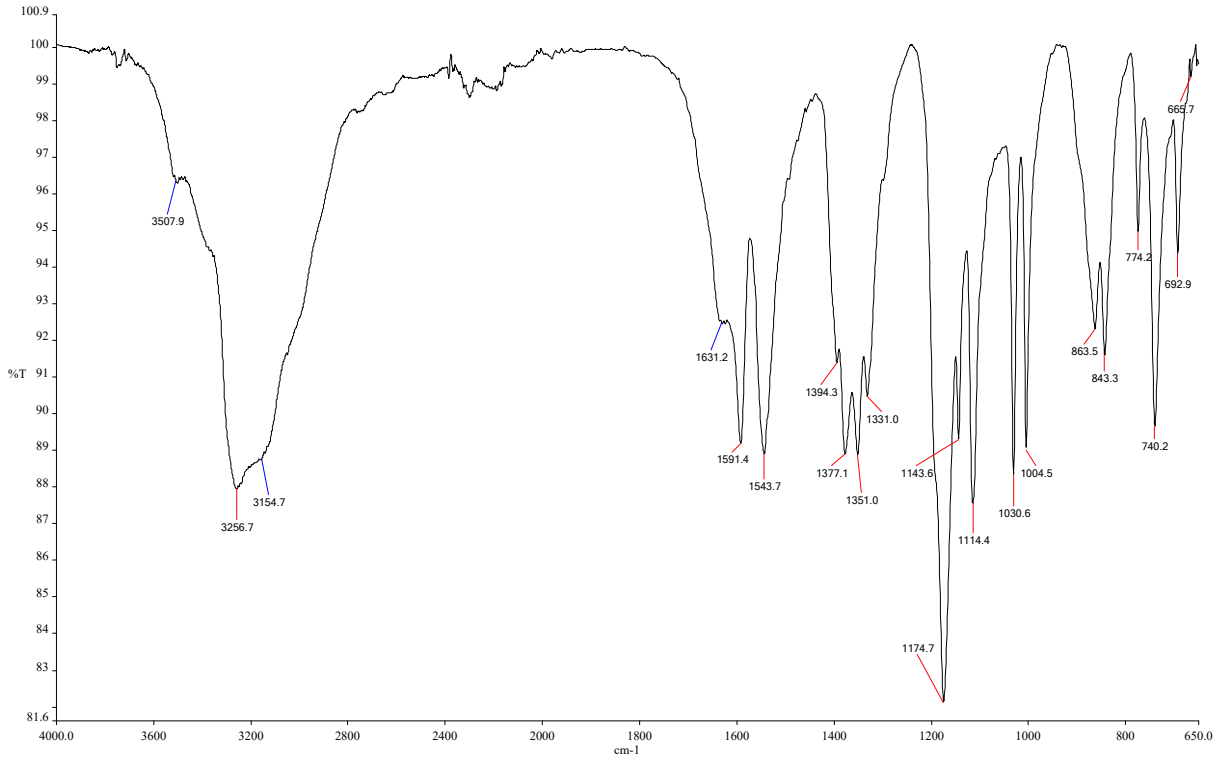


Fig. S7. IR spectrum of $\{[Co(NH_3)_6][K_2(4\text{-sb})_2Cl]\}_n$ (**6**).

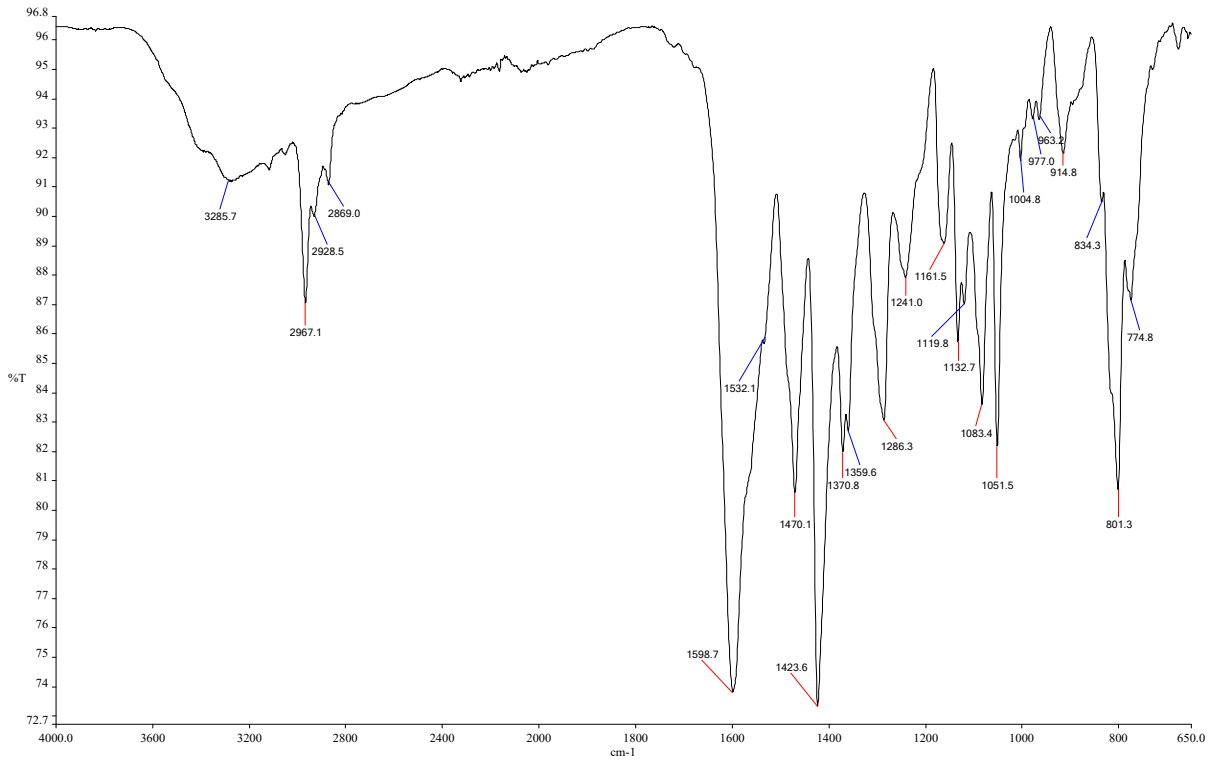
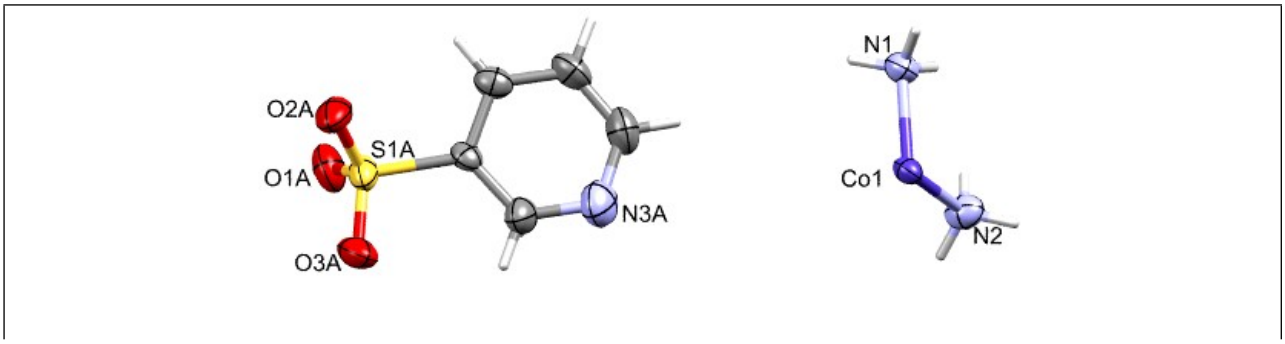
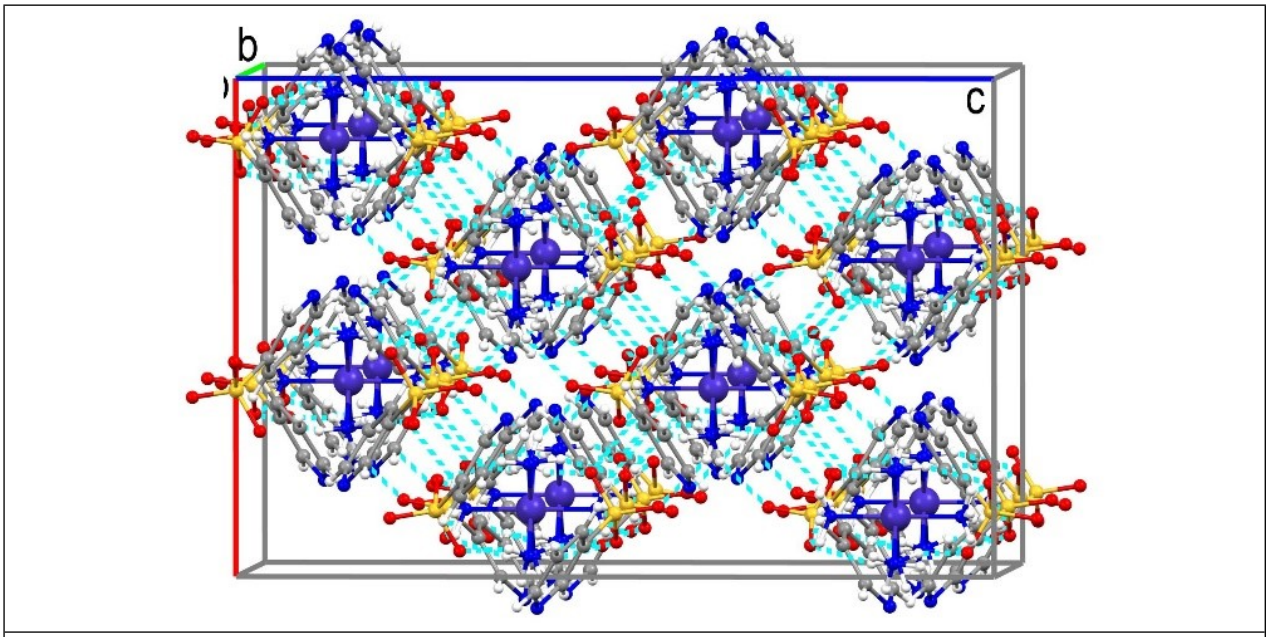


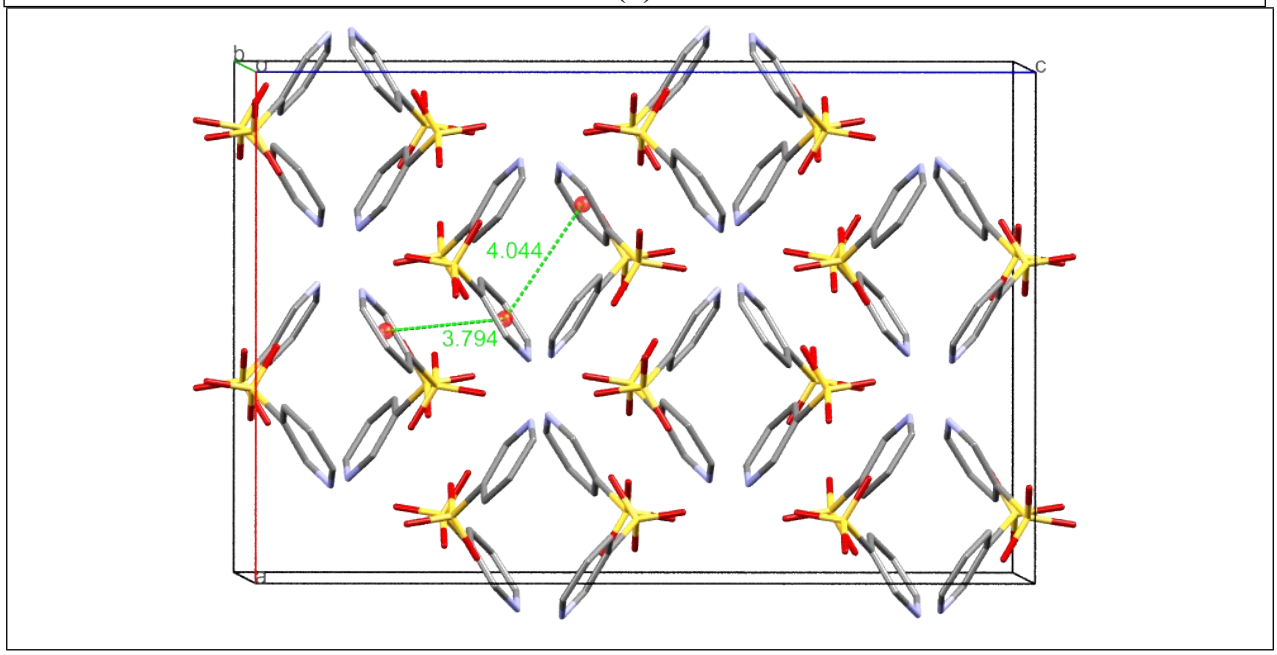
Fig. S8. IR spectrum of $[Co(NH_3)_6](Hssz)(ssz)\cdot 4H_2O$ (**7**).



(a)



(b)



(c)

Fig. S9. (a) The asymmetric unit with thermal ellipsoids shown at 50% probability levels. (b) A fragment of crystal packing in **1**, view along the *c* axis. Hydrogen bonds are shown as blue dotted lines. (c) View of π···π stacking interactions between pyridine moieties in **1**. $[Co(NH_3)_6]^{3+}$ cations are omitted for clarity.

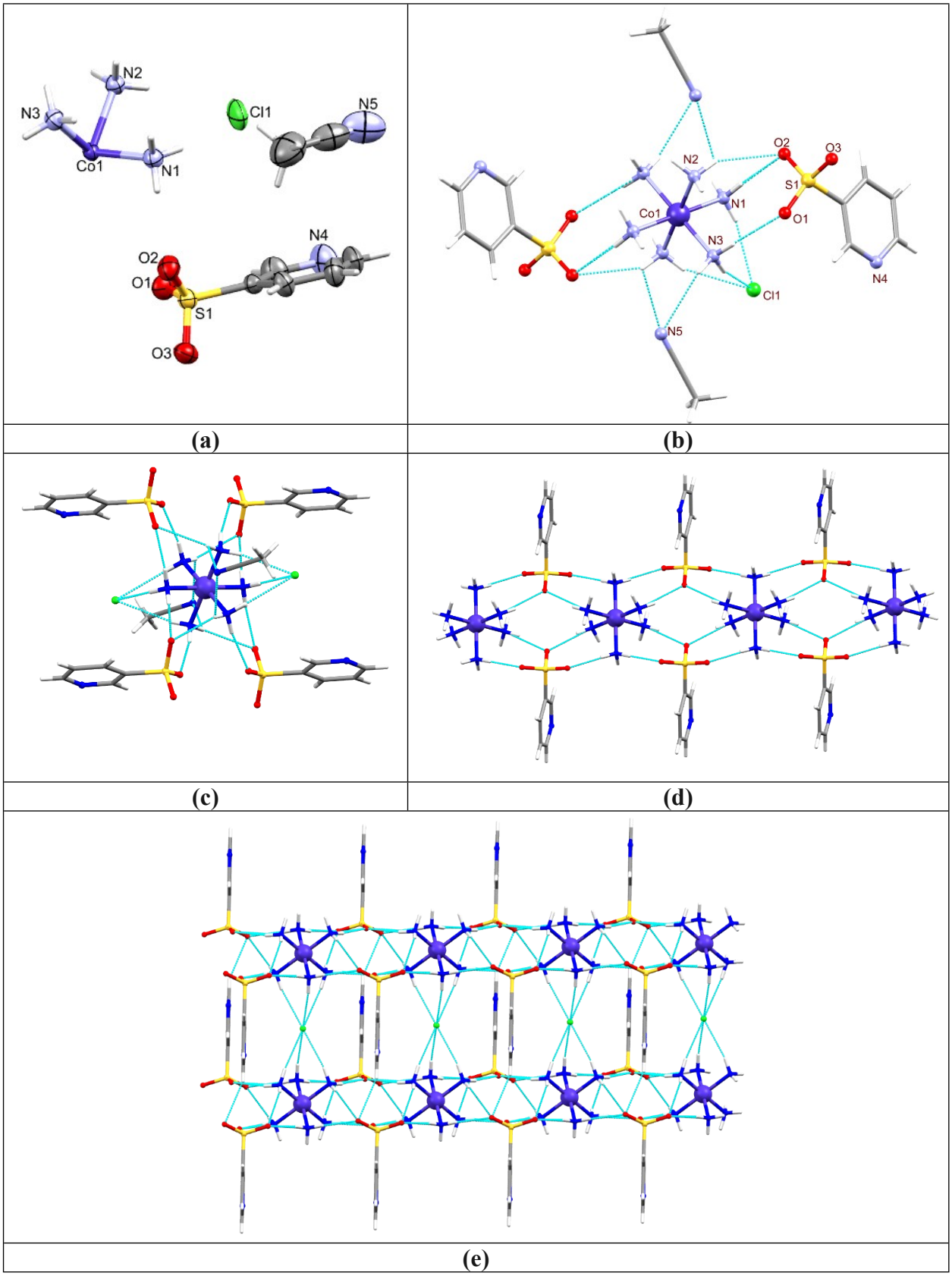


Fig. S10. (a) The asymmetric unit with thermal ellipsoids shown at 50% probability levels. (b) Structure of **2** with a partial numbering. (c) H-bonding interactions around a $[Co(NH_3)_6]^{3+}$ cation in the structure of **2**. (d) A view of 1D hydrogen-bonded chain formed between $[Co(NH_3)_6]^{3+}$cations and pys^- anions. (e) A view of 2D hydrogen-bonded layer formed in **2**. Hydrogen bonds are shown as blue dashed lines.

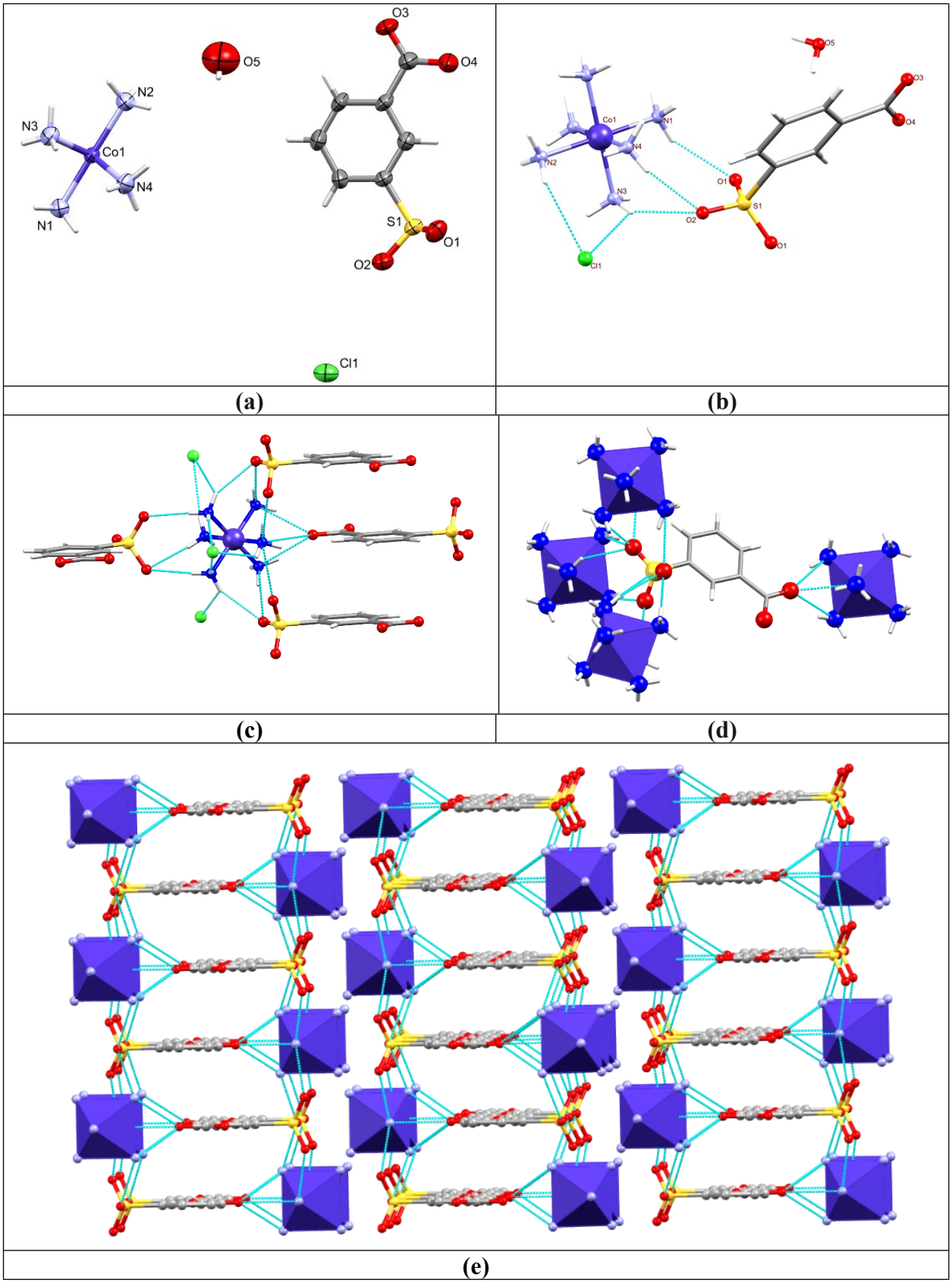
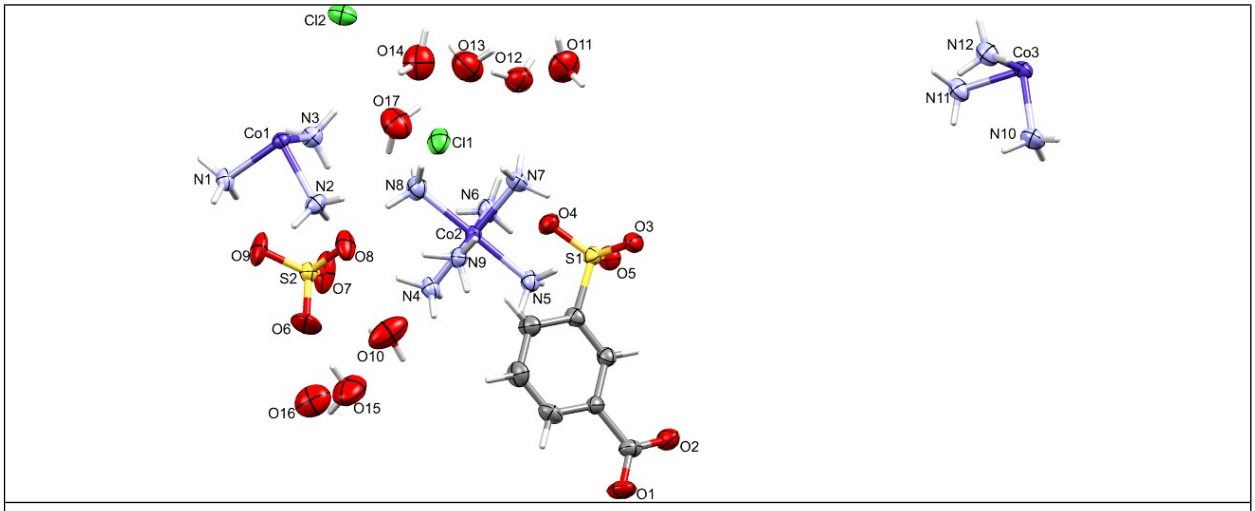
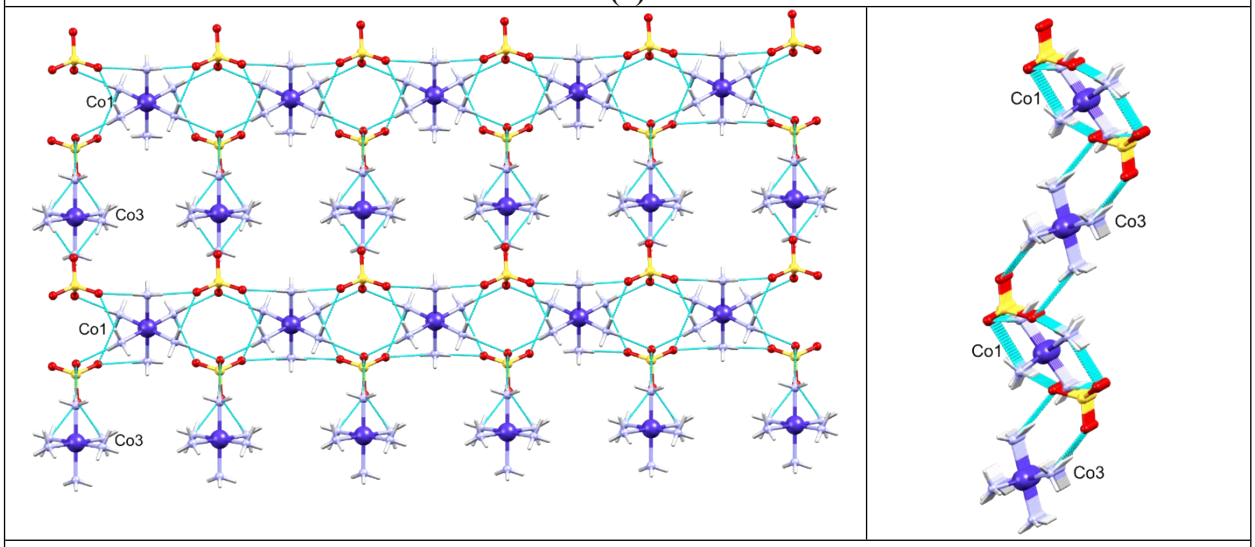


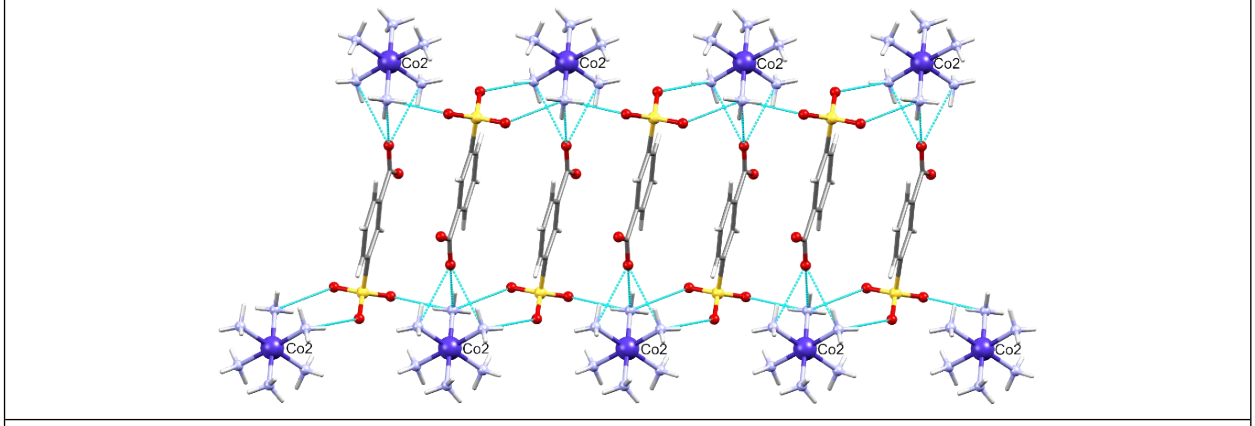
Fig. S11. (a) The asymmetric unit with thermal ellipsoids shown at 50% probability levels. (b) The components of **3** with a partial numbering. (c) H-bonding interactions around $[Co(NH_3)_6]^{3+}$ cation and (d) H-bonding interactions around 3-sb^{2-} dianion. (e) A view of hydrogen-bonded layer of $[Co(NH_3)_6]^{3+}$ cations and 3-sb^{2-} anions in **3**. Co atoms are shown in polyhedron representation. Hydrogen atoms are omitted for clarity. Hydrogen bonds are shown as blue dashed lines.


Cl2
O14
O13
O12
O11
O17
Cl1
N3
Co1
N1
N2
N8
N6
N7
O4
O3
Co2
N9
S1
O5
O9
O8
S2
O7
N4
N5
O6
O10
O16
O15
O2
O1
N12
Co3
N11
N10

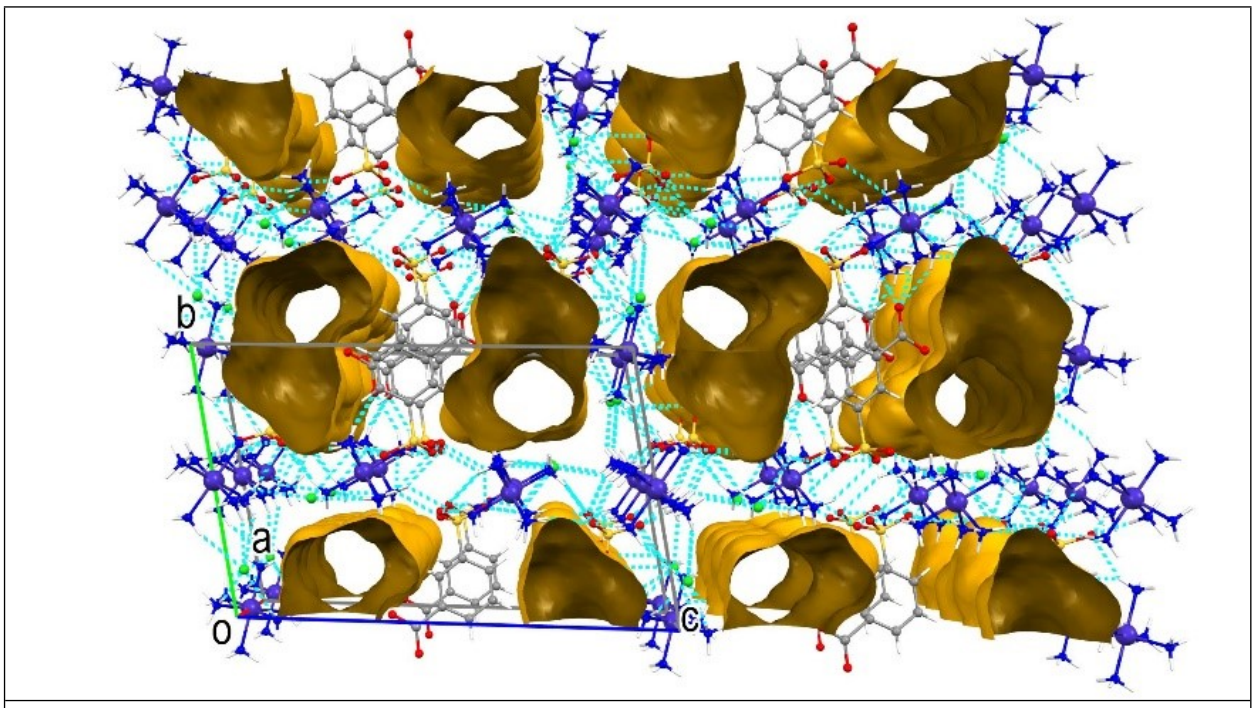
(a)


Co1
Co3
Co1
Co3
Co1
Co3
Co1
Co3

(b)


Co2
Co2
Co2
Co2
Co2
Co2
Co2
Co2
Co2

(c)



(d)

Fig. S12. (a) The asymmetric unit with thermal ellipsoids shown at 50% probability levels. (b) View of a 2D hydrogen-bonded layer formed between Co(III) hexaammine cations (Co1 and Co3) and SO_4^{2-} anions in **4**, and (c) 1D hydrogen-bonded chain formed between Co(III) hexaammine cations (Co2) and 3-sb^{2-} anions. (d) Channels formed by H-bonded charged components in **4** filled by water solvent molecules. Hydrogen bonds are shown as blue dashed lines.

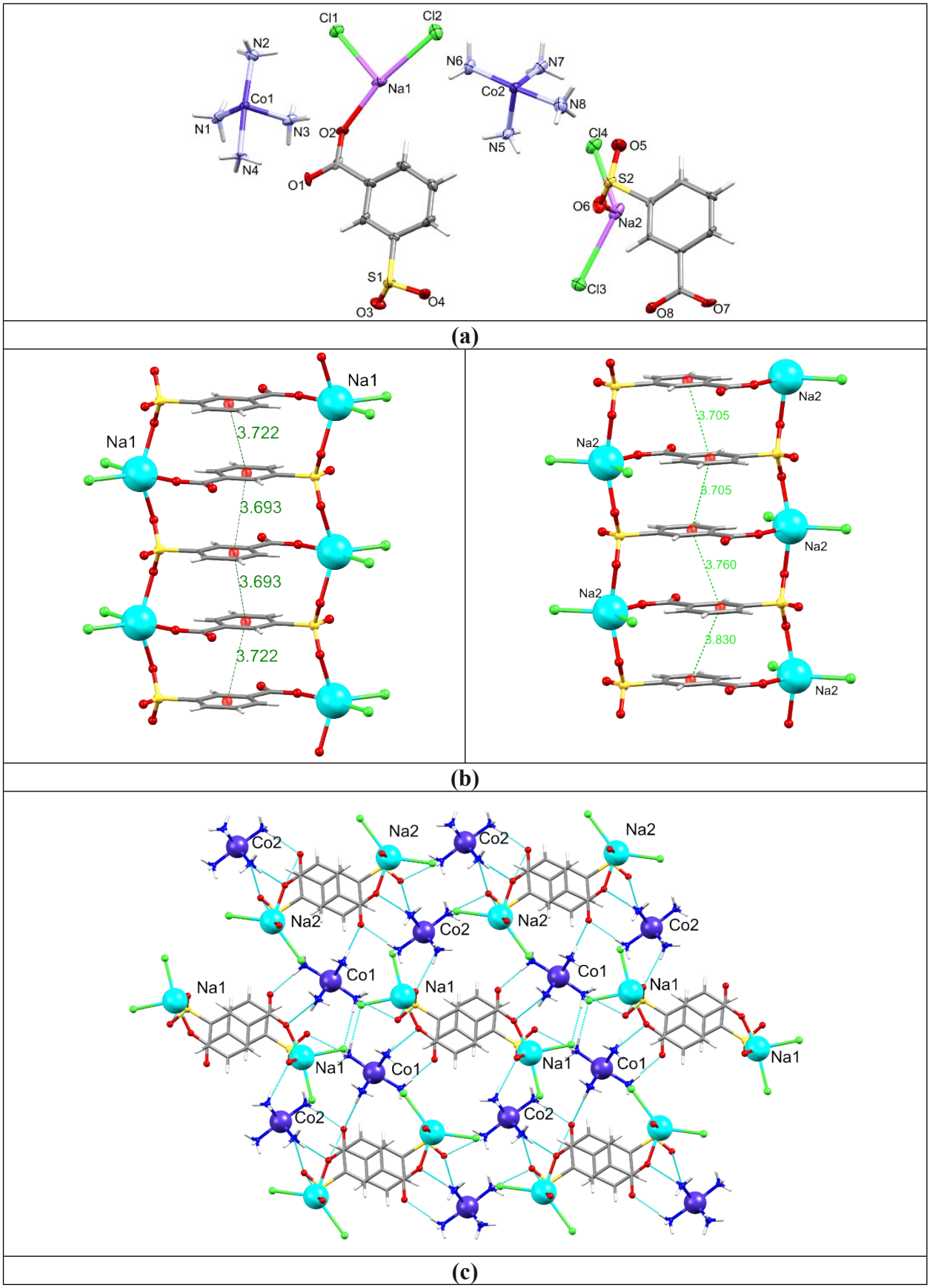


Fig. S13. (a) The asymmetric unit with thermal ellipsoids shown at 50% probability levels. (b) View of a negatively charged $[Na(3\text{-sb})Cl_2]^{3-}$ double-stranded chain in **5**. (c) 3D hydrogen-bonded network formed between $[Na(3\text{-sb})Cl_2]^{3-}$ double-stranded chains and $[Co^{III}(NH_3)_6]^{3+}$ cations. Hydrogen bonds are shown as blue dashed lines.

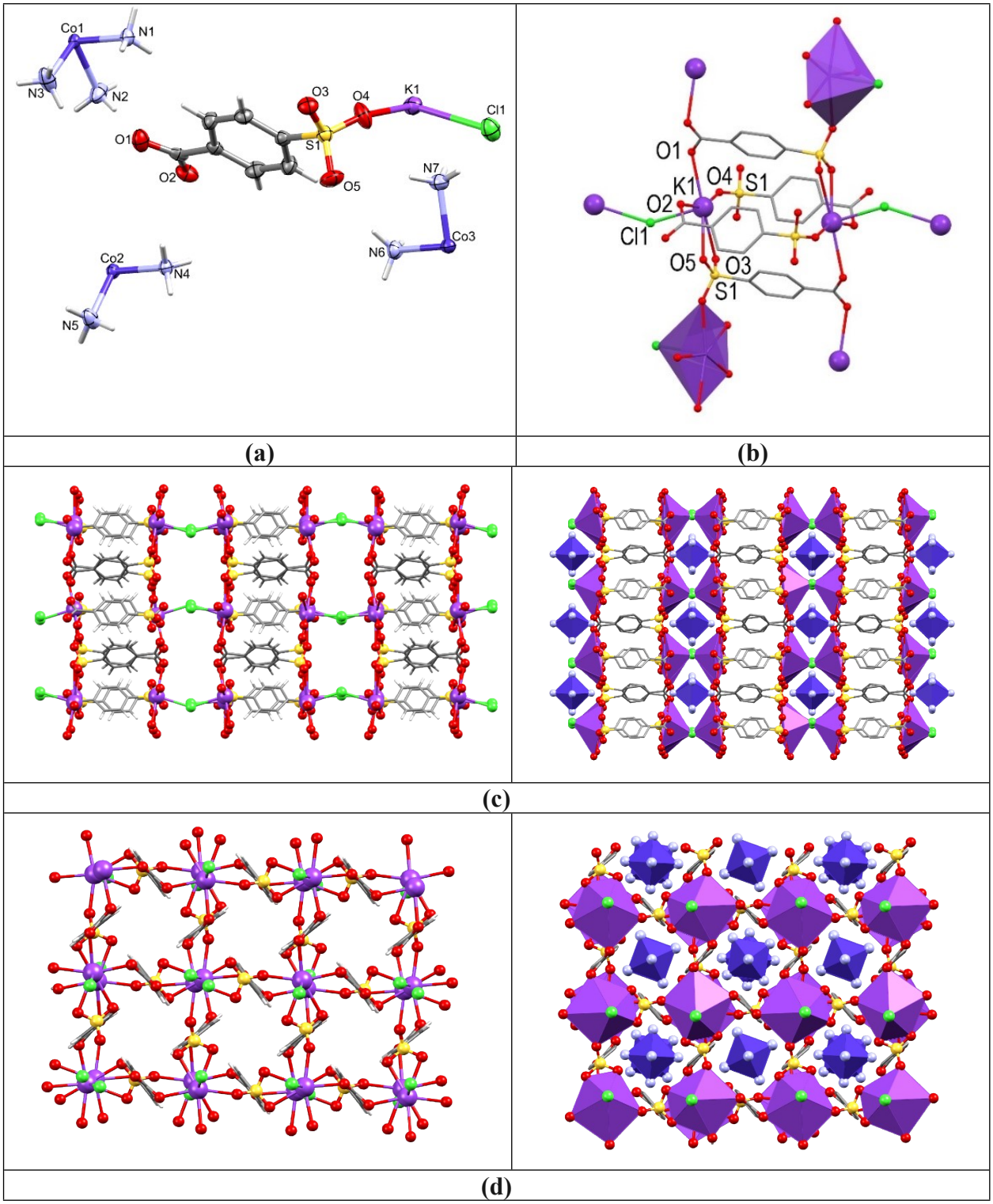
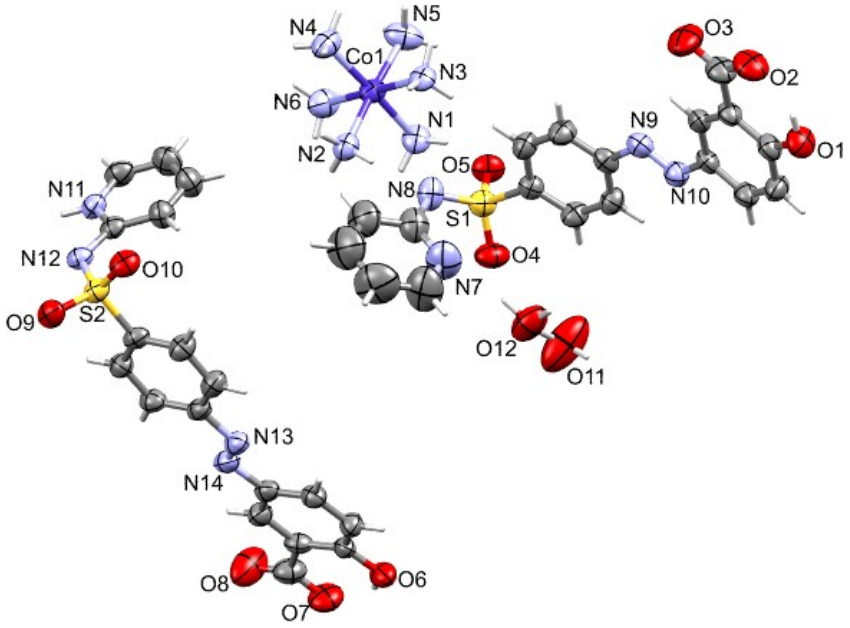
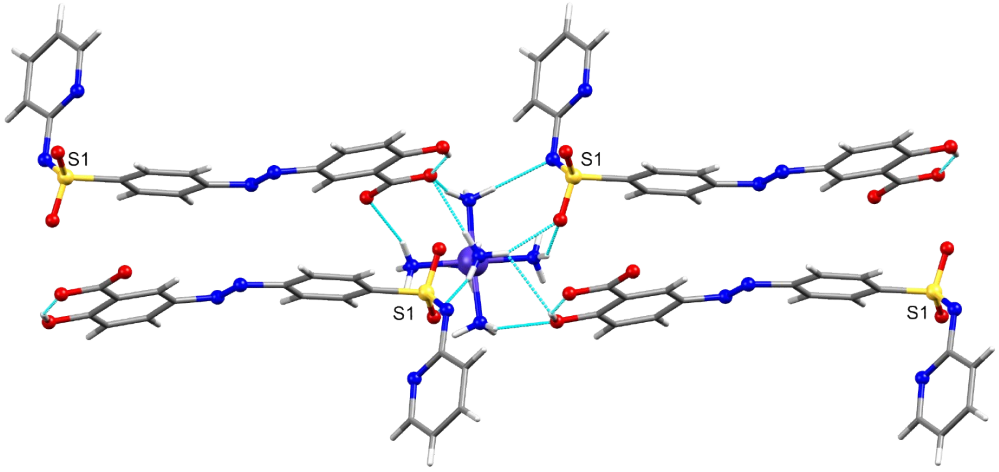


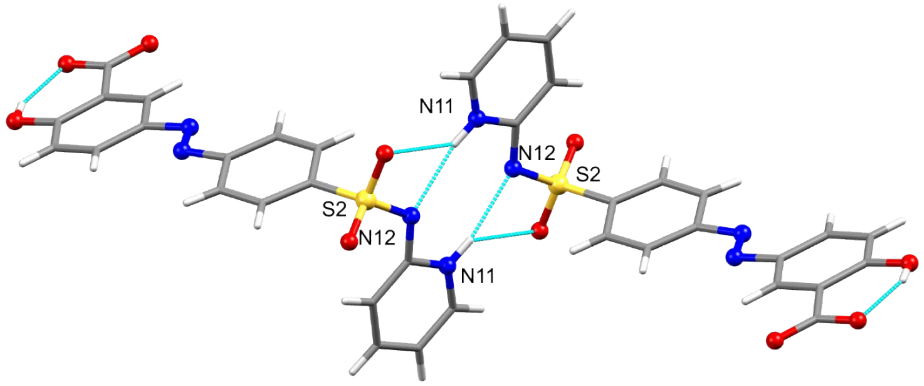
Fig. S14. (a) The asymmetric unit with thermal ellipsoids shown at 50% probability levels. (b) Coordination surrounding of potassium atom in **6**. (c) View of the negatively charged $[K_2(4\text{-sb})_2Cl]^{3-}$ 3D open networks along the *b* axis (left) whose channels contain the $[Co^{III}(NH_3)_6]^{3+}$ cations (right, metal atoms are shown in polyhedral presentation, H atoms are omitted for clarity) in **6**. (d) View of the negatively charged $[K_2(4\text{-sb})_2Cl]^{3-}$ 3D open networks along the *c* axis (left) whose channels contain the $[Co^{III}(NH_3)_6]^{3+}$ cations (right, metal atoms are shown in polyhedral presentation, H atoms are omitted for clarity) in **6**.


N4
N5
Co1
N3
N6
N1
N2
O3
O2
O1
N9
N10
O5
N8
S1
O4
N7
O12
O11
N11
N12
O10
O9
S2
N13
N14
O8
O6
O7

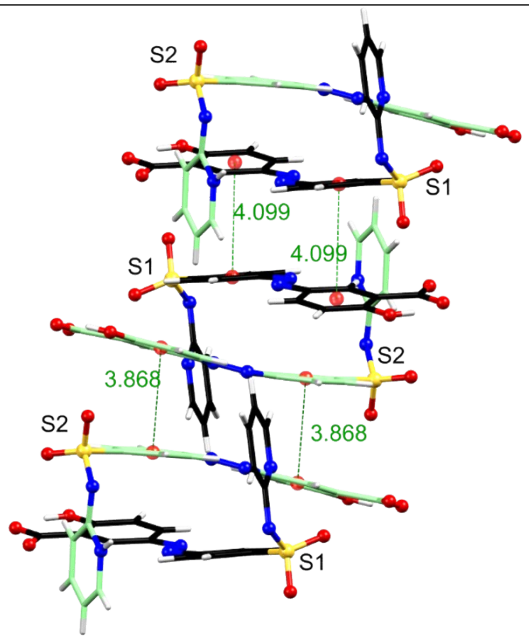
(a)


S1
S1
S1
S1

(b)

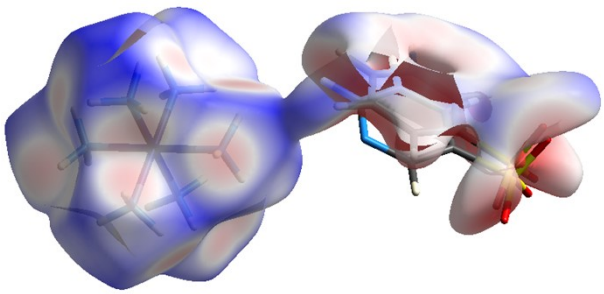

N11
N12
S2
S2
N12
N11

(c)

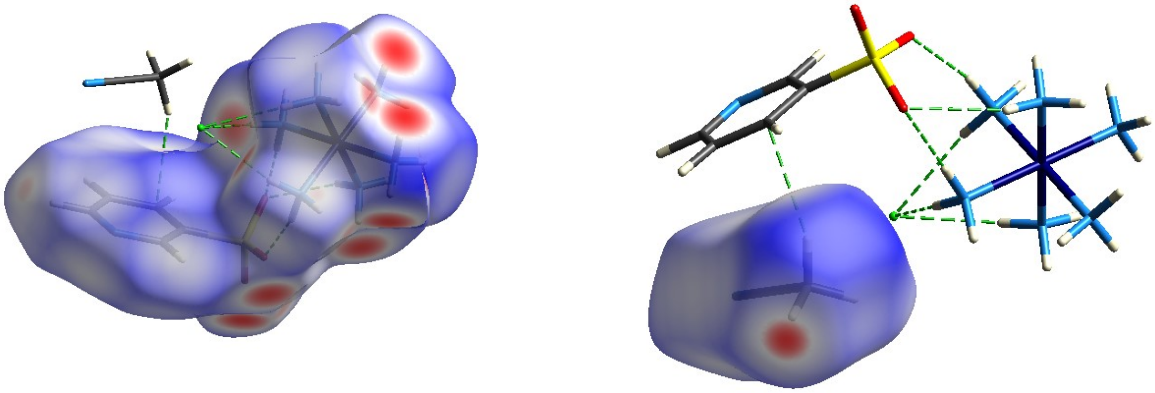


(d)

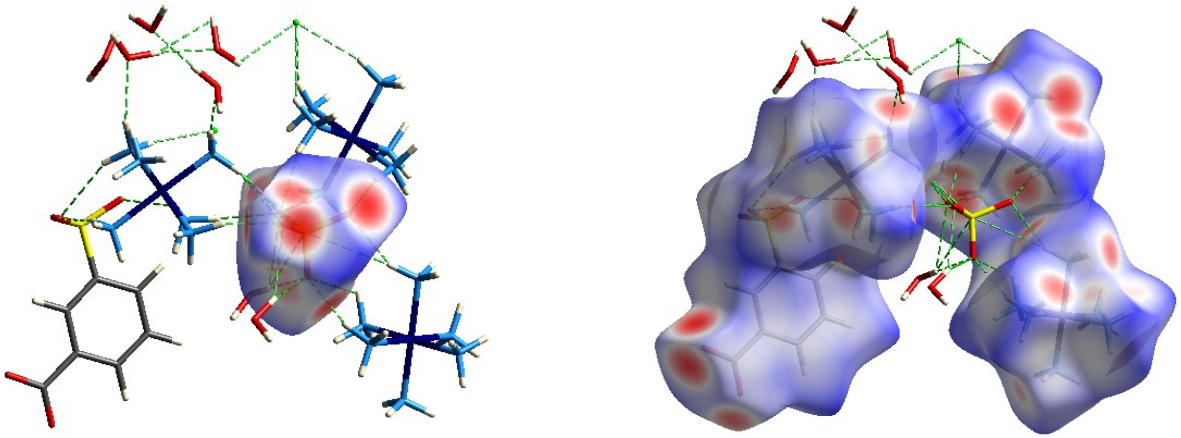
Fig. S15. (a) The asymmetric unit with thermal ellipsoids shown at 50% probability levels. (b) H-bonding interactions around $[Co^{III}(NH_3)_6]^{3+}$ cation (c) H-bonded dimers of $Hssz^-$ monoanions in the structure of **7**. Hydrogen bonds are shown as blue dashed lines. (d) The π···π stacking interactions between $Hssz^-$ moieties (centroid-centroid distance of 3.868 Å, C atoms shown as green sticks) and ssz^{2-} moieties (centroid-centroid distance of 4.099 Å, C atoms shown as black sticks).



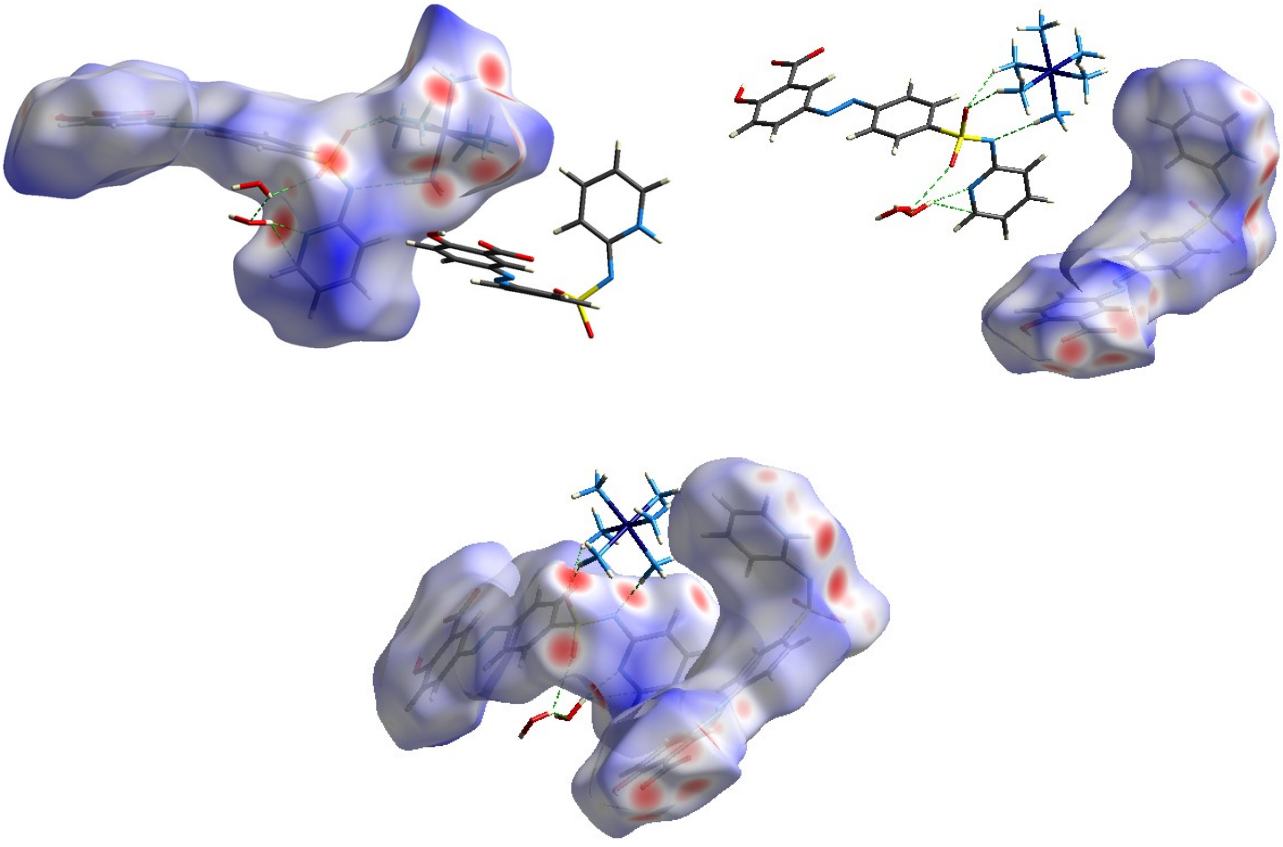
$[Co(NH_3)_6](pys)_3 \cdot Hpys$ (**1**)



$[Co(NH_3)_6](pys)_2Cl \cdot 2MeCN$ (**2**)

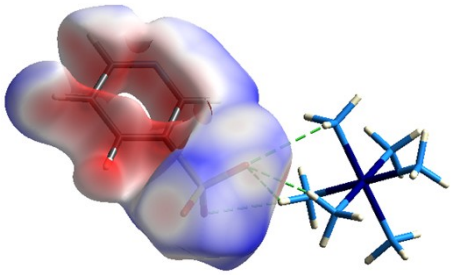


$[Co(NH_3)_6](3\text{-sb})(SO_4)Cl_2 \cdot 7H_2O$ (**4**)

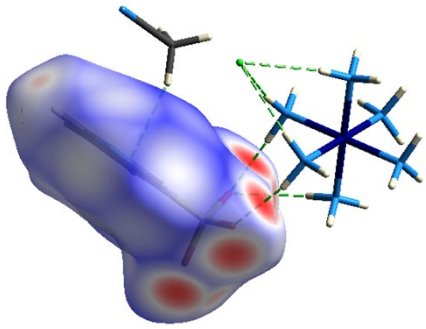


$[Co(NH_3)_6](Hssz)(ssz) \cdot 2H_2O$ (**7**)

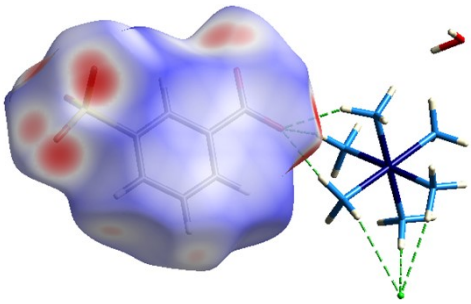
Fig. S16. Hirshfeld surface mapped with d_{norm} property of $[Co(NH_3)_6]^{3+}$ cations and organic or inorganic moieties highlighting close contacts (red areas) with neighbouring molecules in compounds **1**, **2**, **4** and **7**.



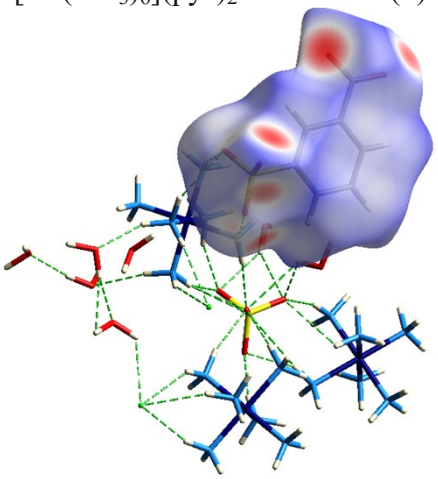
$[Co(NH_3)_6](pys)_3 \cdot Hpys$ (**1**)



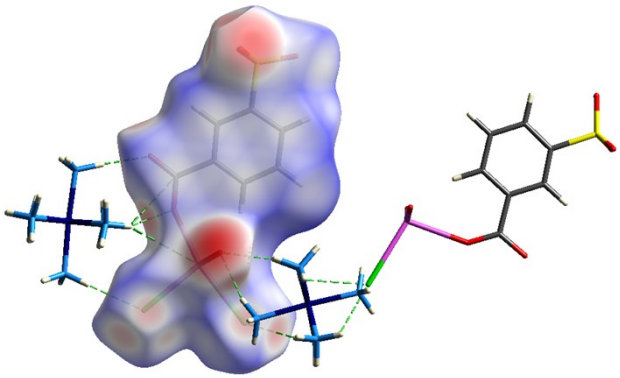
$[Co(NH_3)_6](pys)_2Cl \cdot 2MeCN$ (**2**)



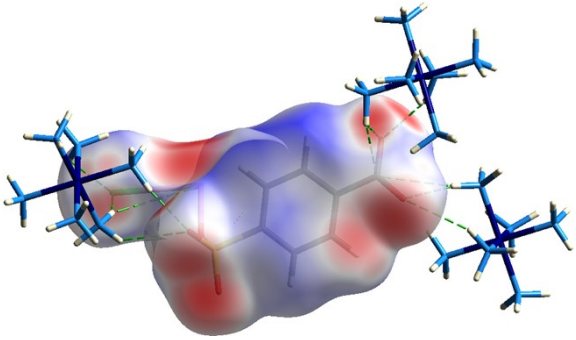
$[Co(NH_3)_6](3\text{-sb})Cl \cdot 4H_2O$ (**3**)



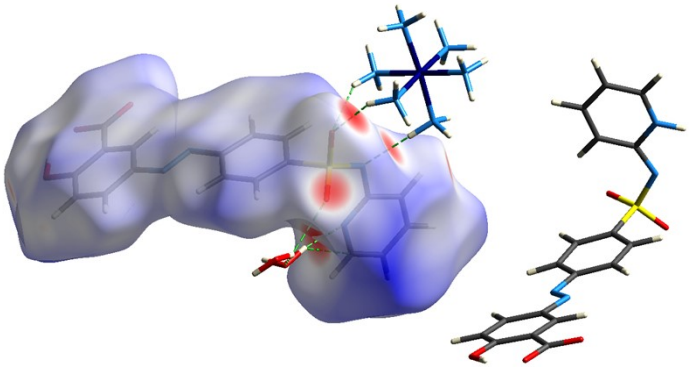
$[Co(NH_3)_6](3\text{-sb})(SO_4)Cl_2 \cdot 7H_2O$ (**4**)



$\{[Co(NH_3)_6][Na(3\text{-sb})Cl_2] \cdot H_2O\}_n$ (**5**)

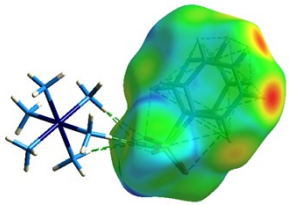
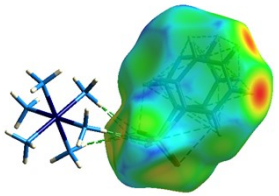
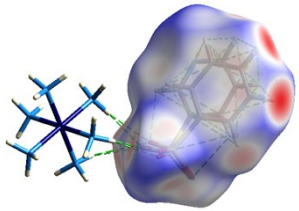
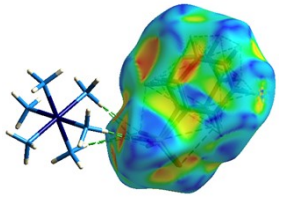
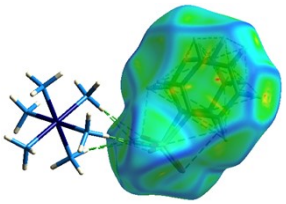
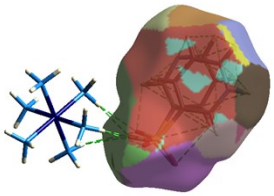
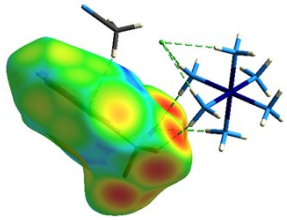
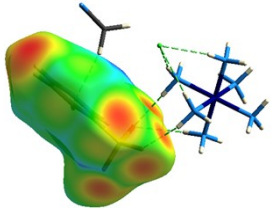
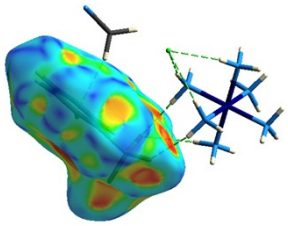
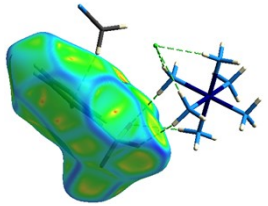
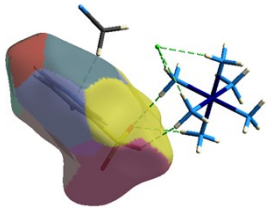
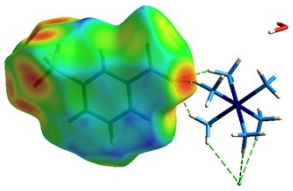
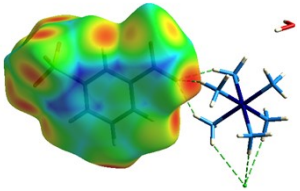
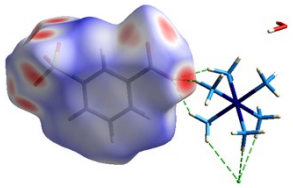
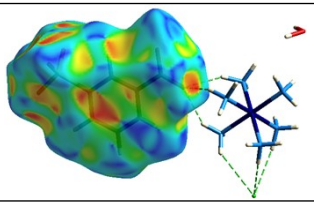
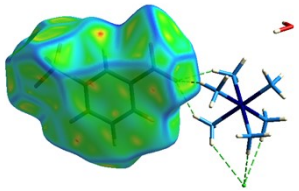
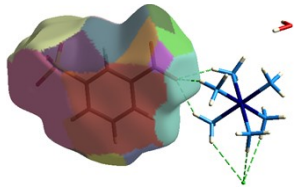
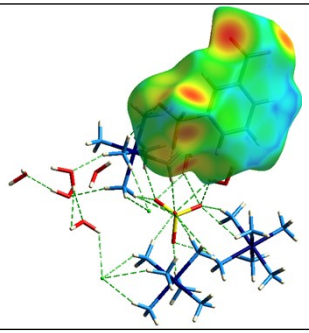
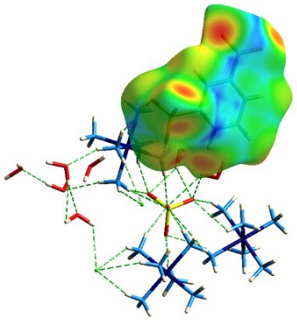
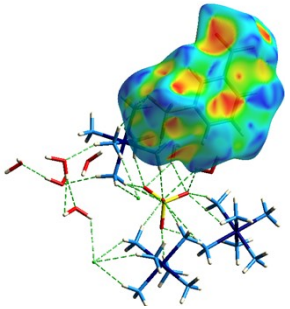
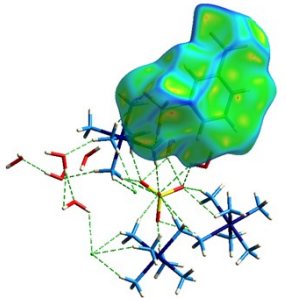
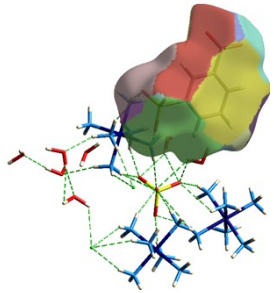


$\{[Co(NH_3)_6][K_2(4\text{-sb})_2Cl]\}_n$ (**6**)



$[Co(NH_3)_6](Hssz)(ssz) \cdot 4H_2O$ (**7**)

Fig. S17. Hirshfeld surface mapped with d_{norm} property of organic moieties highlighting close contacts (red areas) with neighboring $[Co(NH_3)_6]^{3+}$ cations in compounds **1**-**7**.

	d_e	d_i	d_{norm}	shape index	curvedness	fragment patch
1						
2						
3						
4						

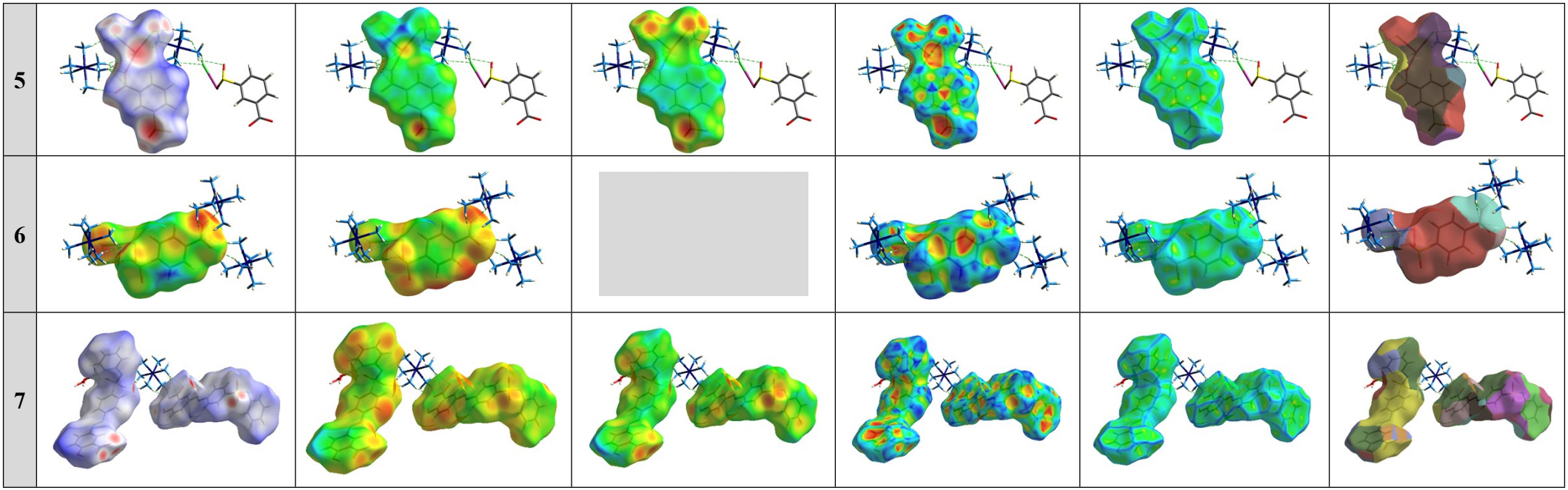
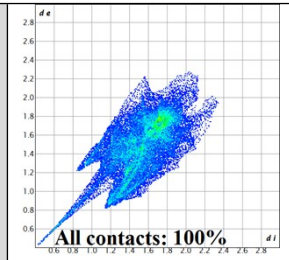
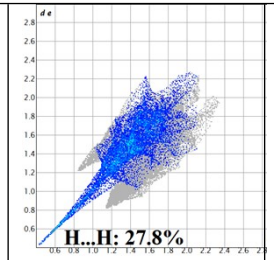
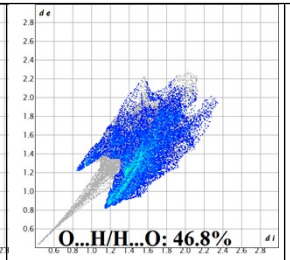
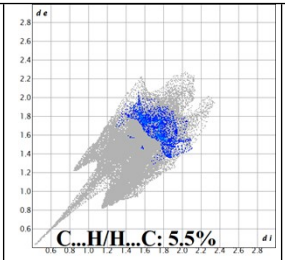
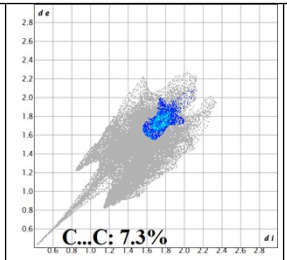
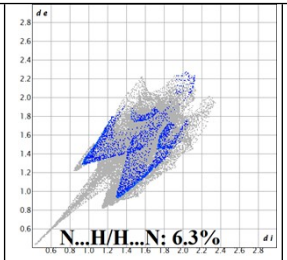
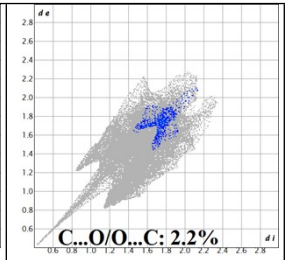
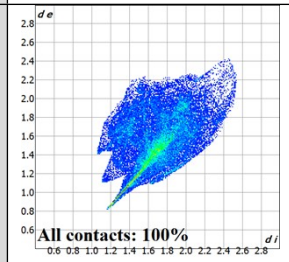
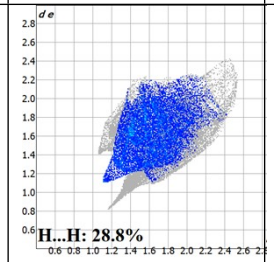
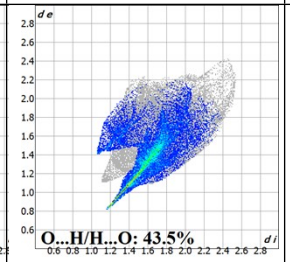
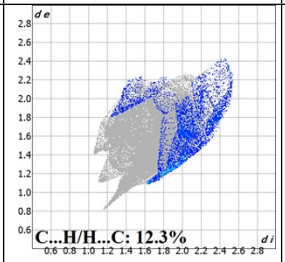
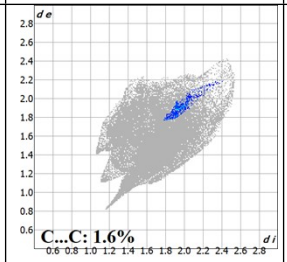
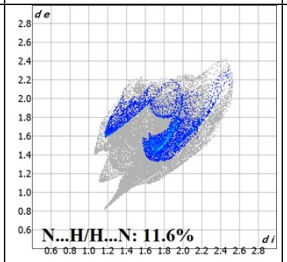
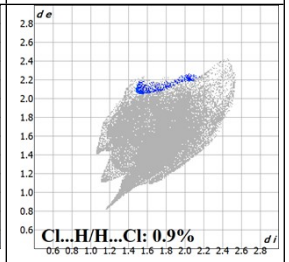
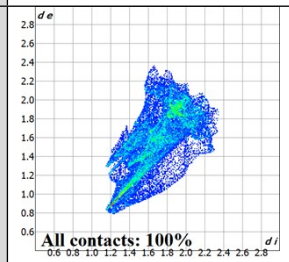
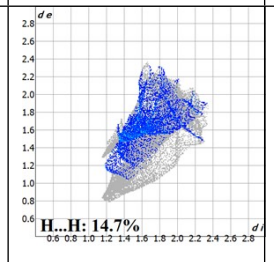
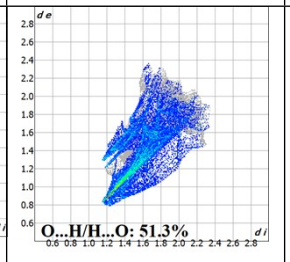
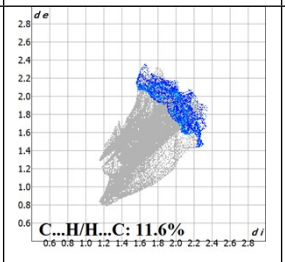
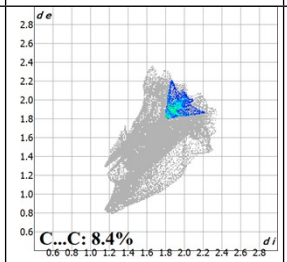
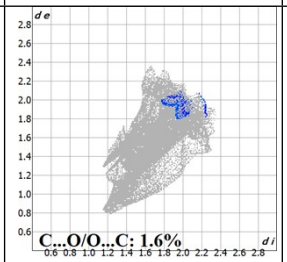
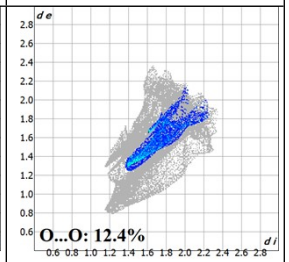
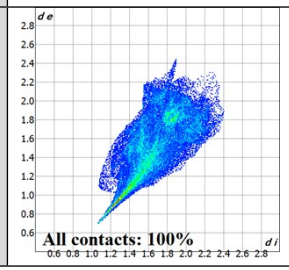
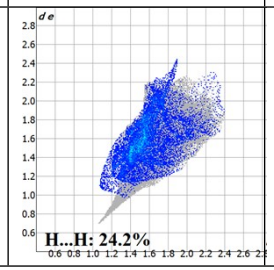
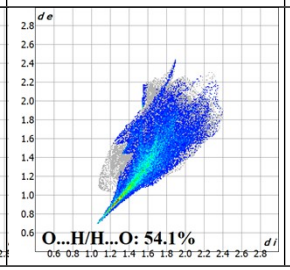
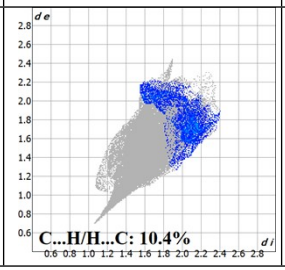
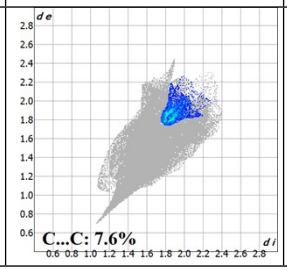
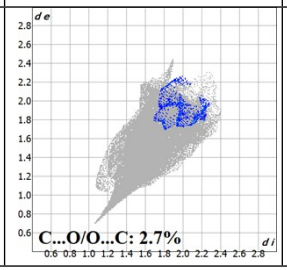
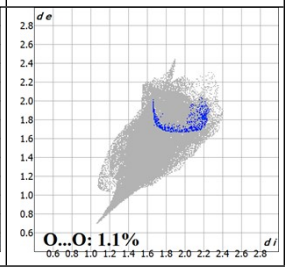


Fig. S18. Hirshfeld surface for organic moieties in **1**-**7** decorated with different properties.

1	 All contacts: 100%	 H...H: 27.8%	 O...H/H...O: 46.8%	 C...H/H...C: 5.5%	 C...C: 7.3%	 N...H/H...N: 6.3%	 C...O/O...C: 2.2%
2	 All contacts: 100%	 H...H: 28.8%	 O...H/H...O: 43.5%	 C...H/H...C: 12.3%	 C...C: 1.6%	 N...H/H...N: 11.6%	 Cl...H/H...Cl: 0.9%
3	 All contacts: 100%	 H...H: 14.7%	 O...H/H...O: 51.3%	 C...H/H...C: 11.6%	 C...C: 8.4%	 C...O/O...C: 1.6%	 O...O: 12.4%
4	 All contacts: 100%	 H...H: 24.2%	 O...H/H...O: 54.1%	 C...H/H...C: 10.4%	 C...C: 7.6%	 C...O/O...C: 2.7%	 O...O: 1.1%

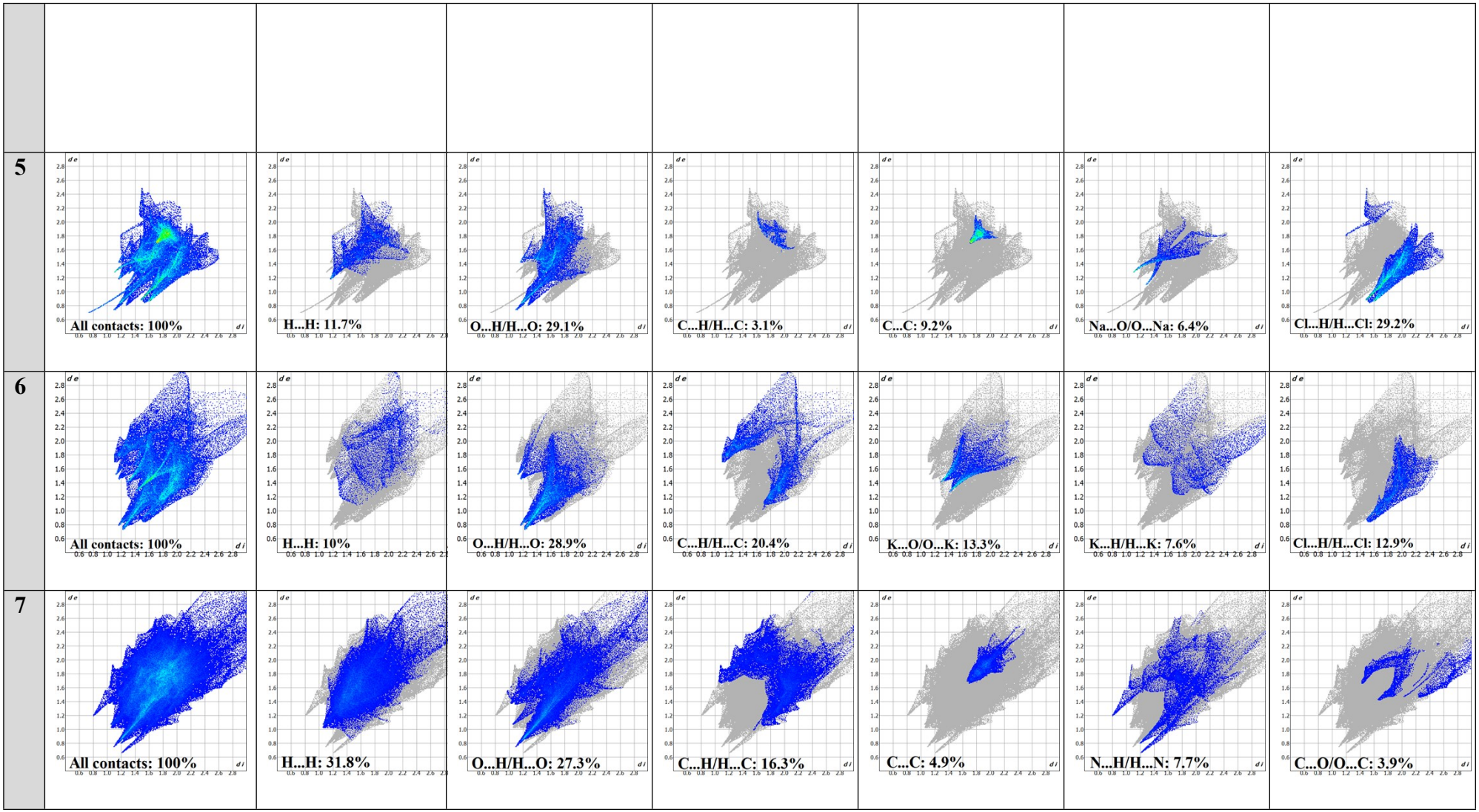
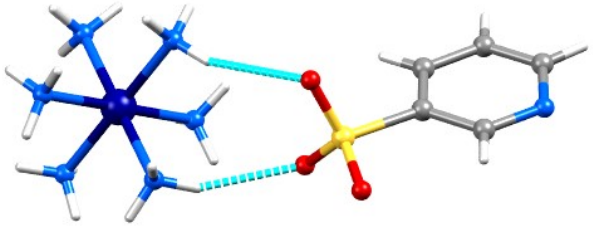
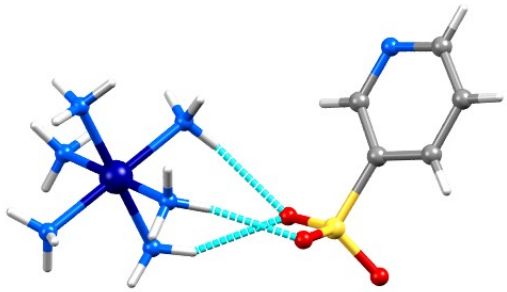


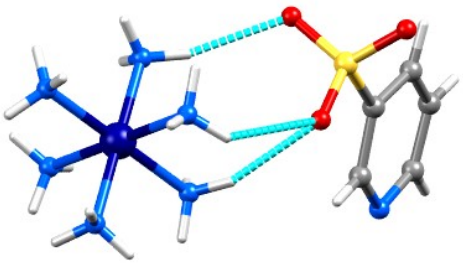
Fig. S19. 2D fingerprint plots for all and individual contacts in crystal packing of **1**-**7**.



(a)

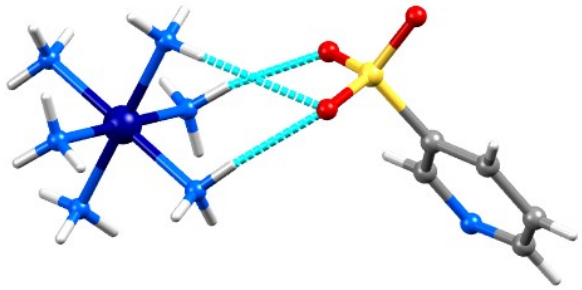


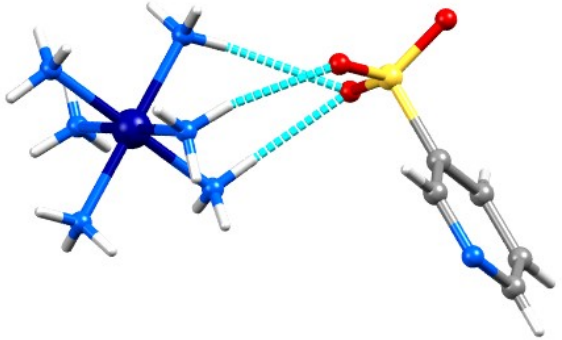
(b)



(c)

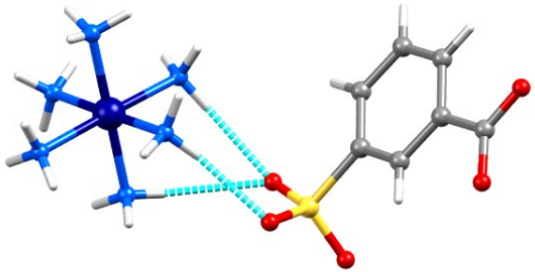
$[Co(NH_3)_6]^{3+} \cdot (pys)^-$ (**1**)

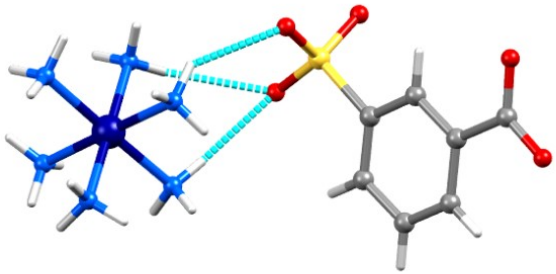




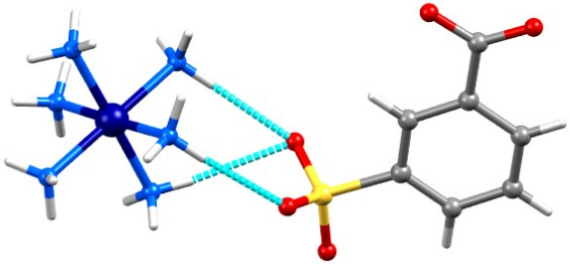
(a) **(b)**

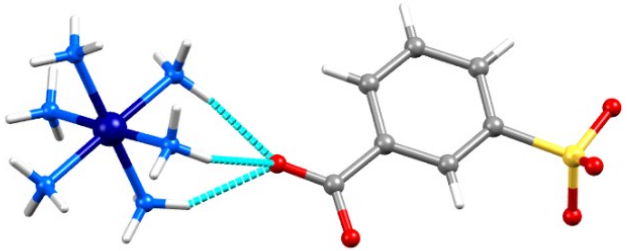
$[Co(NH_3)_6]^{3+} \cdot (pys)^{-}$ (**2**)





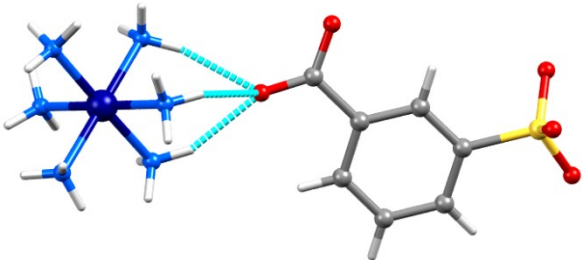
(a) **(b)**

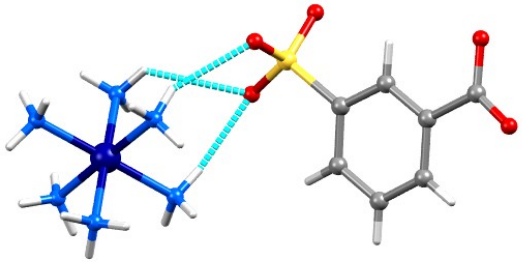


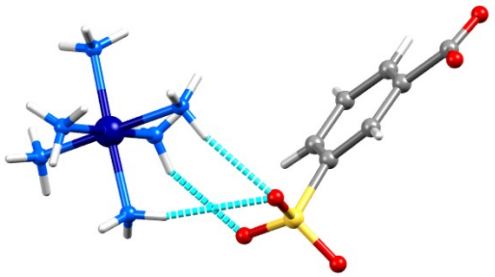


(c) **(d)**

$[Co(NH_3)_6]^{3+} \cdot (sb)^{2-}$ (**3**)

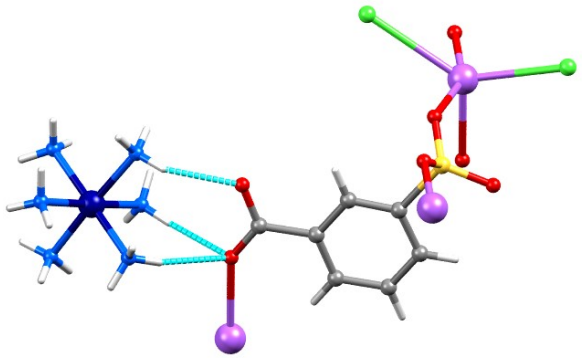






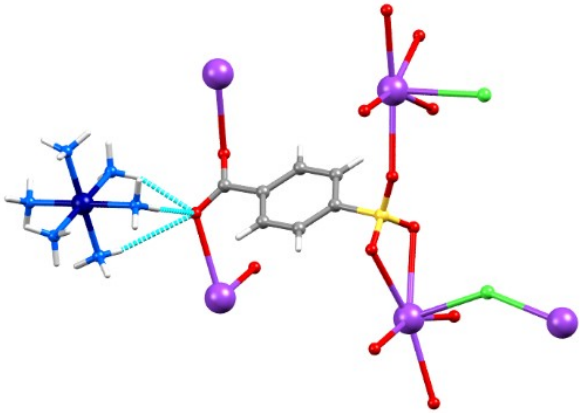
(a) **(b)** **(c)**

$[Co(NH_3)_6]^{3+} \cdot (sb)^{2-}$ (**4**)

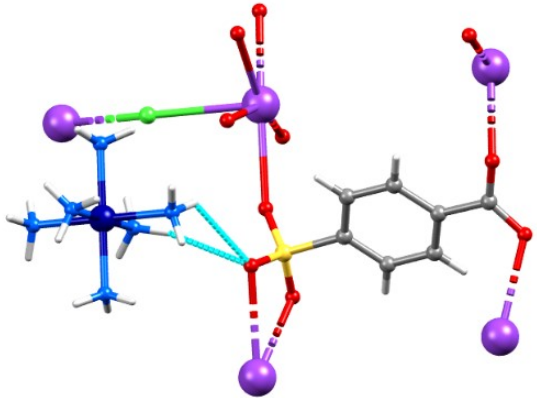


(a)

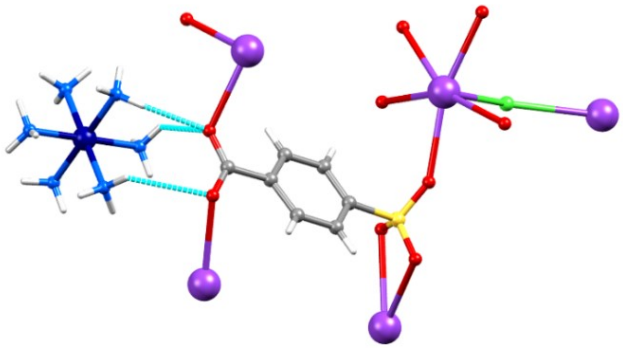
$[Co(NH_3)_6]^{3+} \cdot (sbNa)^{-}$ (**5**)



(a)

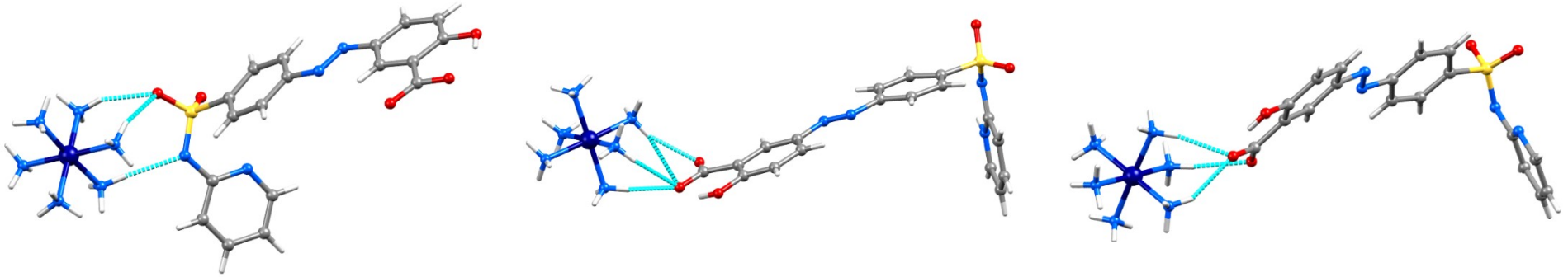


(b)



(c)

$[Co(NH_3)_6]^{3+} \cdot (sbK)^{-}$ (**6**)



(a) **(b)** **(c)**

$[Co(NH_3)_6]^{3+} \cdot (ssz)^{2-}$ (**7**)

Fig. S20. View of all selected pairs for estimation of their interaction energies in **1**-**7**.